
NBS MONOGRAPH 25— SECTION 14

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

# Standard X-ray Diffraction Powder Patterns

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.

[2] Located at Boulder, Colorado 80302.

# Standard X-ray Diffraction Powder Patterns
# Section 14—Data for 68 Substances



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Issued September 1977

Library of Congress Catalog Card Number: 53-61386

National Bureau of Standards Monograph 25
Section 14—Data for 68 Substances
Nat. Bur. Stand. (U.S.), Monogr. 25—Sec. 14, 143 pages (Sept. 1977)
CODEN: NBSMA6

U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1977

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402
Price $2.75. Stock No. 003–003–01842–2

CONTENTS

## ERRATA

A book has been published containing card images of NBS Standard X-ray Diffraction Powder Patterns[1]. During preparation of the book, some errors were found and corrected on the card images. A list of them is available on request. The corrections below are in addition to those included on the card images.

Circular 539

Vol. 1, p. 67 Density should be 2.749 $g/cm^3$
1, p. 78 In the test for chemical analysis, the word should be "thiocyanate."
2, p. 28 Previous erratum (Mono. 25, Sec. 5) changed the space group to Ia3. Change also the following indices: for d = 2.068, 1.808, 1.491, 1.1646, and 1.1110, use hkℓ = 431, 433, 543, 833, and 851 respectively.
3, p. 27 Previous erratum (Mono. 25, Sec. 5) changed the space group to Ia3. Change also the following indices: for d = 1.9301, 1.6885, and 1.3924, use hkℓ = 431, 433, and 543 respectively.
4, p. 67 In the lattice constants, the NBS values for "b" and "c" should be interchanged. Because "b" and "c" are so nearly equal, a few indices may also need to be changed.
5, p. 30 At hkℓ = 321, "d" should be 1.4479. At hkℓ = 631, "d" should be 0.7987.
6, p. 41 Delete "$CdI_2$-type structure." Insert "$K_2GeF_6$ is used as a structure type."
10, p. 4 Formula in title should be $AlPO_4$.

Monograph 25

Sec. 5, p. 11 At hkℓ = 002, d should be 4.401.
11, p. 39 Add this structural information: "The cubic cell given with Z = ½ is a pseudo-cell. The true cell with Z = 1 has random voids in the Hg position."
12, p. iii The formula for magnesium titanium oxide should be $Mg_2TiO_4$.
12, p. 42 The text and the references at the end should both have the year 1975 for the reference to McMurdie et al.
13, p. 26 At d = 1.648, the hkℓ's should be $\bar{4}42$,530.
13, p. 36 At d = 2.423, the intensity should be 20.
13, p. 79 Density should be 8.605.

[1]Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081, $150.00).

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## STANDARD X-RAY DIFFRACTION POWDER PATTERNS

The following copies may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia, 22161. Where these publications are identified with a number, it must be used in ordering. They are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

Also, until the present supply is exhausted, the publication numbers marked by an asterisk are for sale from the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402. Order Sections 11, 12, and 13 respectively, by catalog no. SN 003-003-01234-3, $1.55; SN 003-003-01376-5, $1.50; or C13.44:25/Sec. 13, $1.80. (Add 25% additional for other than U. S. mailing).

| NBS Publication | Number |
|---|---|
| Circular 539, Volume 1 | PB 178 902 |
| Volume 2 | PB 178 903 |
| Volume 3 | PB 178 904 |
| Volume 4 | PB 178 905 |
| Volume 5 | PB 178 906 |
| Volume 6 | PB 178 907 |
| Volume 7 | PB 178 908 |
| Volume 8 | PB 178 909 |
| Volume 9 | PB 178 910 |
| Volume 10 | PB 178 911 |

| NBS Publication | Number |
|---|---|
| Monograph 25, Section 1 | PB 178 429 |
| Section 2 | PB 178 430 |
| Section 3 | PB 178 431 |
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| Section 6 | |
| Section 7 | |
| Section 8 | PB 194 872 |
| Section 9 | COM 72-50002 |
| Section 10 | COM 72-51079 |
| *Section 11 | COM 74-50183 |
| *Section 12 | COM 75-50162 |
| *Section 13 | |

# STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 14. --- Data for 68 Substances

by

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Standard x-ray diffraction patterns are presented for 68 substances. Twenty-seven of these patterns represent experimental data and 41 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

## INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,[1] the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 68 compounds (27 experimental and 41 calculated patterns), and is the twenty-fourth of the series of "Standard X-ray Diffraction Powder Patterns."[2]

## EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data. In some cases, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with sample lines, silver or silicon was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid errors associated with aberrations at the very top of peaks, the readings of $2\theta$ were taken at positions about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction for each region was then applied to the measured value of $2\theta$. We have reported all data as $K\alpha_1$ peaks because the internal standard corrections for all regions were established in terms of the $K\alpha_1$ wavelength.

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[1]Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, PA. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

[2]See previous page for other published volumes.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in the table below; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Calculated 2θ Angles, CuKα$_1$ λ = 1.540598Å

| hkℓ | W a=3.16524Å ±.00004 | Ag a=4.08651Å ±.00002 | Si a=5.43088Å ±.00004 |
|---|---|---|---|
| 110 | 40.262 | | |
| 111 | | 38.112 | 28.443 |
| 200 | 58.251 | 44.295 | |
| 211 | 73.184 | | |
| 220 | 86.996 | 64.437 | 47.303 |
| 310 | 100.632 | | |
| 311 | | 77.390 | 56.123 |
| 222 | 114.923 | 81.533 | |
| 321 | 131.171 | | |
| 400 | 153.535 | 97.875 | 69.131 |
| 331 | | 110.499 | 76.377 |
| 420 | | 114.914 | |
| 422 | | 134.871 | 88.032 |
| 511/333 | | 156.737 | 94.954 |
| 440 | | | 106.710 |
| 531 | | | 114.094 |
| 620 | | | 127.547 |
| 533 | | | 136.897 |
| 444 | | | 158.638 |

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for a single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in $10^5$ [Hubbard et al. 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: λ(CuKα$_1$, peak)= 1.540598Å [Deslattes and Henins, 1973].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the *International Tables for X-ray Crystallography, Vol. I* [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of *Crystal Data* [1973]. For primitive cells, the transformed cell axes are an alternate labelling of the reduced cell axes. For centered monoclinic cells, the transformed cell is the centered cell with the three shortest non-coplanar vectors.

A computer program [Evans et al., 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. In indexing cubic patterns, multiple hkℓ's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number $6.0220943 \times 10^{23}$ [Deslattes et al., 1974] and atomic weights published by IUPAC [1972].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical

position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. Any intensity larger than 20 was rounded to the nearer multiple of 5. At least 3 patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference Intensity Ratio, $I/I_{corundum}$. The reference intensity ratio, $I/I_c$, has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113(hexagonal) of corundum [Visser and de Wolff, 1964]. The ratio is tabulated for copper K$\alpha$ radiation, for a 1:1 mixture by weight of the sample and corundum.

A new procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum, $x_s$ and $x_c$ ($x_s = 1-x_c$), intensities $I(\underline{h})$ and $I(\underline{k})$ are measured for several sets of reflections $\underline{h}$ and $\underline{k}$, usually within the same region of $2\theta$, to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(\underline{h}_0)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{rel}(\underline{k})}{I^{rel}(\underline{h})} \cdot \frac{I(\underline{h})}{I(\underline{k})}$$

and $(\underline{h}_0)$ indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection $(\underline{h}_0)$ will be the one with I=100 since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, $I/I_c$. These values yield the tabulated average $\langle I/I_c \rangle$. From these data, an estimated standard deviation, $\Delta$, (given in parentheses), was obtained from

$$\Delta = \frac{\sum_{i=1}^{n} \left| (I/I_c)_i - \langle I/I_c \rangle \right|}{n}$$

where n is the number of measurements of the reference intensity ratio.

## CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Clark, Smith and Johnson [1973] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made in the lattice constants in order to make them consistent with the revised value of $\lambda(CuK\alpha_1)$= 1.540598Å [Deslattes and Henins, 1973]. Both the altered and the original published values are given. A lattice constant arrangement which follows the conventions of Crystal Data has been referred to as the "CD cell." In several of the calculated patterns, the literature lattice constants, the atom positions, and hence the final patterns were not given in the CD arrangement. For cross-reference purposes, the CD cell was calculated separately and included in the text.

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the *International Tables for X-ray Crystallography, Vol. III*, [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's or the anisotropic $\beta_{ij}$'s in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

$$e^{-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})}.$$

Other thermal parameters were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, instead of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4 \left[ \frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}\, b^{*2}\, c^{*2}} \right]^{\frac{1}{3}}$$

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. In our text, when the expression "the structure was determined by..." was used, the atomic parameters in the reference cited had been calculated from refinement of single crystal data. Otherwise, the atomic positions had been derived by analogy with similar compounds whose structure was known. In cases where isostructural relationships were used, the atoms were in fixed special positions or the ionic radii were closely related to the corresponding radii of the atoms in the known structure.

Integrated intensities. The theoretical integrated intensity of reflection i on the "absolute/relative" scale is computed from the right hand side of the equation:

$$\frac{I_i^{abs}}{K} = \frac{M_i Lp_i |F_i T_i|^2}{2\mu V^2}$$

where:

F is the structure factor
T is the thermal correction

$Lp = \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$ is the Lorentz-polarization term

M is the multiplicity for the reflection i
$\mu$ is the linear absorption coefficient
V is the volume of the unit cell

When the largest integrated intensity was assigned a relative value of 100 and all other reflections were scaled relative to it, the intensities were placed on the relative intensity scale ($I^{rel}$). Relative intensities were rounded to the nearest integer value before being listed, and reflections with $I^{rel}$ less than 0.7 were omitted.

Scale factor (integrated intensities). The scale factor, $\gamma$, was defined to convert the tabulated $I^{rel}$ to the "absolute/relative" scale [Hubbard, Evans and Smith, 1976]. That is:

$$\gamma = \frac{M'Lp'|F'T'|^2}{200\mu V^2}$$

and

$$\frac{I^{abs}}{K} = \gamma I^{rel}$$

The primes denoted the values for the largest integrated intensity. In earlier Monographs (1969-1975), a different scale factor, $k_{NBS}$, was reported which is related to $\gamma$:

$$\frac{\gamma}{k_{NBS}} = \frac{1}{2\mu V^2}$$

From $\gamma$, the theoretical value of the Reference Intensity Ratio, $I/I_c$, was calculated:

$$I/I_c = \frac{\mu\gamma\rho_c}{\mu_c\gamma_c\rho}$$

where $\rho$ is the density and the subscript c represents corundum ($\alpha$-$Al_2O_3$).

For refined structures, the value of $I/I_c$ was given. For those phases whose structures were postulated or were based only on analogy to other powder patterns, $I/I_c$ was not included and any intensity above 20 was rounded further, to the nearer multiple of 5.

$I/I_c$ and $\gamma$ are each based on the single strongest reflection, not on the overlapping sum of superimposed reflections.

Peak intensities. The purpose of calculating peak intensities was to provide a tabulated pattern similar to what might be obtained from experimental diffractometer measurements. For each predicted reflection, Cauchy profiles centered at both the $\alpha_1$ and the $\alpha_2$ peak positions were calculated and summed, forming a simulated powder pattern. The full width at half-maximum (FWHM) was allowed to vary to represent the changing FWHM as a function of 2$\theta$. [The values of the FWHM vs 2$\theta$ are given in the table below]. The resultant simulated powder pattern was then analyzed for peaks. In the regions of the predicted reflections several reflections could have identical or similar 2$\theta$ angles and produce only one composite peak in the simulated pattern. The 2$\theta$ angle of the composite peak was assigned the hk$\ell$ of the reflection having the greatest contribution to the peak intensity. If any other peak contributed more than 10% of the intensity toward the composite peak intensity, a plus sign (+) was appended to the hk$\ell$. Peaks due solely to $\alpha_2$ lines were omitted. If an $\alpha_1$ peak and an $\alpha_2$ peak overlapped, the $\alpha_1$ reflection was listed only when it contributed a significant intensity (>10%) at the peak 2$\theta$.

The peak search routine located peaks only at 2$\theta$ angles which were a multiple of 0.02°.

| 2θ CuKα1 | FWHM | 2θ CuKα1 | FWHM |
|---|---|---|---|
| 0° | 0.12° | 140 | 0.230 |
| 20 | .12 | 145 | .255 |
| 40 | .12 | 150 | .285 |
| 60 | .125 | 155 | .315 |
| 80 | .130 | 160 | .360 |
| 100 | .135 | 162.5 | .410 |
| 120 | .155 | 165 | .500 |
| 130 | .185 | | |

## REFERENCES


Alexander, L., Klug, H. P. and Kummer, E. (1948). J. Appl. Phys., *19*, No. 8, 742.

Clark, C.M., Smith, D.K., and Johnson, G.G., Jr. (1973). A FORTRAN IV Program for Calculating X-ray Powder Diffraction Patterns, Version 5, Dept. of Geosciences, Pennsylvania State Univ., University Park, PA 16802.

*Crystal Data* (1973). (3rd. Ed. Published jointly by the U. S. Department of Commerce, National Bureau of Standards, Washington, D. C. 20234, and the Joint Committee on Powder Diffraction Standards, Swarthmore, PA 19081).

Deslattes, R.D. and Henins, A. (1973). Phys. Rev. Lett. *31*, 972.

Deslattes, R. D., Henins, A., Bowman, H. A., Schoonover, R.M., Carroll, C.L., Barnes, I.L., Machlan, L.A., Moore, L. J., and Shields, W.R. (1974). Phys. Rev. Lett. *33*, 463.

Evans, H.T., Jr., Appleman, D. E. and Handwerker, D.S. (1963), Report #PB 216188, U. S. Dept. of Commerce,National Technical Information Center 5285 Port Royal Rd., Springfield, VA 22151, $3.50.

Hartshorne, N.H. and Stuart, A. (1970). *Crystals and the Polarizing Microscope* (Edward Arnold and Co., London, 4th Ed.)

Hubbard, C. R., Evans, E. H., and Smith, D. K. (1976). J. Appl. Cryst., *9*, 169.

Hubbard, C. R. and Smith, D. K. (1977). *Advances in X-ray Analysis*, *20*, (to be published).

Hubbard, C. R., Swanson, H. E., and Mauer, F. A. (1975). J. Appl. Cryst. *8*, 45.

*International Tables for X-ray Crystallography, I* (1952). (The Kynoch Press, Birmingham, Eng.), Ibid. *III* (1962). Pgs. 202, 210, 213, 214.

International Union of Pure and Applied Chemistry (1972). Pure Appl. Chem. *30*, Nos. 3-4, 639.

ISCC-NBS Centroid Color Charts, SRM 2106 (1965), obtainable from the Office of Standard Reference Materials, Room B311, Chemistry Building, National Bureau of Standards, Washington, D.C. 20234. $5.00 per set.

Palache, C., Berman, H. and Frondel, C. (1944). *Dana's System of Mineralogy* (John Wiley and Sons, New York, 7th Ed.), *I*, 6.

Standard Reference Material 640, Silicon Powder, X-ray Diffraction Standard, obtainable from the Office of Standard Reference Materials, Room B311, Chemistry Building, National Bureau of Standards, Washington, D.C. 20234. $52.00 per 10 gram unit.

Swanson, H. E., Morris, M. C., and Evans, E. H. (1966). Nat'l Bur. Std. U.S. Monograph 25, Sec. *4*, 3.

Visser, J.W. and de Wolff, P.M. (1964). "Absolute Intensities," Report 641.109, Technisch Physische Dienst, Delft, Netherlands.

# Ammonium iron chloride hydrate, $(NH_4)_2FeCl_5 \cdot H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an acid aqueous solution of $NH_4Cl$ and $FeCl_3$.

Color
Deep reddish orange

Optical Data
Biaxial (+), $N_\alpha = 1.755$, $N_\beta = 1.77$, $N_\gamma = 1.82$. 2V is large.

Structure
Orthorhombic, Pmnb (62), Z=4, isostructural with $K_2FeCl_5 \cdot H_2O$ (erythrosiderite) [Bellanca, 1947]. The structure of $(NH_4)_2FeCl_5 \cdot H_2O$ was determined by Lindqvist [1946, 1948].

NBS lattice constants of this sample:

a = 9.925(3) Å
b = 13.713(3)
c = 7.039(2)

Volume
957.9 $Å^3$

Density
(calculated) 1.991 $g/cm^3$

Reference intensity
$I/I_{corundum} = 0.8$

References
Bellanca, A., (1947). Ric. Sci. Ricostr. 17, 1360.
Lindqvist, I., (1946). Ark. Kemi Mineral. Geol. A24, No. 1.
Lindqvist, I., (1948). Acta Chem. Scand. 2, 530.

$CuK\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.26 | 8 | 011 | 14.13 |
| 5.74 | 100 | 101 | 15.43 |
| 5.64 | 95 | 120 | 15.71 |
| 5.29 | 9 | 111 | 16.73 |
| 4.96 | 60 | 200 | 17.87 |
| 4.92 | 80 | 021 | 18.03 |
| 4.39 | 5 | 121 | 20.19 |
| 4.01 | 6 | 220 | 22.13 |
| 3.836 | 12 | 031 | 23.17 |
| 3.579 | 5 | 131 | 24.86 |
| 3.515 | 5 | 002 | 25.32 |
| 3.492 | 4 | 221 | 25.49 |
| 3.426 | 6 | 040 | 25.99 |
| 3.410 | 4 | 012 | 26.11 |
| 3.082 | 17 | 041 | 28.95 |
| 3.034 | 18 | 231 | 29.42 |
| 2.989 | 25 | 122 | 29.87 |
| 2.983 | 25 | 320 | 29.93 |
| 2.945 | 12 | 141 | 30.32 |
| 2.869 | 35 | 202 | 31.15 |
| 2.820 | 95 | 240 | 31.70 |
| 2.812 | 85 | 212 | 31.80 |
| 2.787 | 65 | 032 | 32.09 |
| 2.742 | 4 | 321 | 32.63 |
| 2.685 | 5 | 132 | 33.34 |
| 2.648 | 5 | 222 | 33.83 |
| 2.617 | 4 | 241 | 34.24 |
| 2.557 | 4 | 051 | 35.07 |
| 2.481 | 65 | 400 | 36.17 |
| 2.456 | 50 | 042 | 36.55 |
| 2.432 | 4 | 232 | 36.93 |
| 2.382 | 5 | 142,340 | 37.73 |
| 2.313 | 11 | 013 | 38.91 |
| 2.308 | 9 | 411 | 38.99 |
| 2.227 | 4 | 160 | 40.47 |
| 2.214 | 20 | 421 | 40.73 |
| 2.202 | 12 | 242 | 40.96 |
| 2.174 | 11 | 061 | 41.50 |
| 2.163 | 15 | 052 | 41.73 |
| 2.114 | 13 | 152 | 42.73 |
| 2.082 | 11 | 431 | 43.42 |
| 2.042 | 19 | 133 | 44.32 |
| 1.991 | 6 | 261 | 45.53 |
| 1.984 | 4 | 252 | 45.68 |
| 1.932 | 7 | 441 | 46.99 |
| 1.907 | 10 | 520 | 47.66 |
| 1.881 | 8 | 162,360 | 48.34 |
| 1.854 | 25 | 171,432 | 49.10 |
| 1.811 | 6 | 352 | 50.34 |
| 1.782 | 7 | 053 | 51.22 |
| 1.764 | 5 | 271 | 51.78 |
| 1.745 | 25 | 442,014 | 52.40 |
| 1.7180 | 13 | 540 | 53.28 |
| 1.7150 | 8 | 512,080 | 53.38 |
| 1.6915 | 8 | 413 | 54.18 |
| 1.6696 | 6 | 541 | 54.95 |
| 1.6654 | 5 | 081 | 55.10 |
| 1.6429 | 8 | 181,034 | 55.92 |
| 1.6346 | 8 | 461 | 56.23 |
| 1.6304 | 9 | 452 | 56.39 |
| 1.6201 | 6 | 280,134 | 56.78 |
| 1.5434 | 5 | 542,314 | 59.88 |

# Ammonium potassium iron chloride hydrate, (kremersite) $(NH_4,K)_2\ FeCl_5 \cdot H_2O$

Sample

The sample was prepared by slow evaporation at room temperature of a 1:1:1 molar aqueous solution of $NH_4Cl$, KCl and $FeCl_3$. The first crystals formed were used. From a plot of the cell parameters of the end members of the solid solution series, this sample was determined to be close to a 1:1 molar ratio of $NH_4$ to K. This is similar to the reported analysis of the natural mineral, kremersite, from Mt. Vesuvius [Palache et al., 1951].

Color

Deep reddish orange

Structure

Orthorhombic, Pmnb (62), Z=4, isostructural with $K_2FeCl_5 \cdot H_2O$ and $(NH_4)_2FeCl_5 \cdot H_2O$. The structure of $K_2FeCl_5 \cdot H_2O$ was determined by Bellanca[1947].

NBS lattice constants of this sample

a = 9.808(3)Å
b = 13.657(4)
c = 7.028(2)

Volume

941.4

Density

(calculated) 2.175 g/cm$^3$.

Reference Intensity

$I/I_{corundum} = 1.2$

References


Bellanca, A. (1947). Ric. Sci. Ricostr. 17, 1360.

Palache, C., Berman, H., and Frondel, C. (1951). Dana's System of Mineralogy (John Wiley & Sons, New York, 7th Ed.) pg. 101.


$CuK\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.72 | 80 | 101 | 15.48 |
| 5.61 | 55 | 120 | 15.78 |
| 5.270 | 7 | 111 | 16.81 |
| 4.900 | 40 | 200,021 | 18.09 |
| 3.820 | 6 | 031 | 23.27 |
| 3.464 | 7 | 221 | 25.70 |
| 3.411 | 9 | 040 | 26.10 |
| 3.070 | 16 | 041 | 29.06 |
| 3.016 | 17 | 231 | 29.60 |
| 2.966 | 13 | 301 | 30.11 |
| 2.951 | 9 | 320 | 30.26 |
| 2.857 | 25 | 202 | 31.28 |
| 2.800 | 100 | 240 | 31.93 |
| 2.794 | 60 | 212 | 32.00 |
| 2.783 | 55 | 032 | 32.14 |
| 2.601 | 4 | 241 | 34.45 |
| 2.548 | 3 | 051 | 35.20 |
| 2.451 | 65 | 400,042 | 36.64 |
| 2.374 | 4 | 142 | 37.86 |
| 2.310 | 4 | 013 | 38.95 |
| 2.277 | 2 | 060 | 39.54 |
| 2.191 | 11 | 421,242 | 41.16 |
| 2.157 | 12 | 052 | 41.84 |
| 2.106 | 9 | 152 | 42.91 |
| 2.038 | 14 | 133 | 44.41 |
| 1.889 | 7 | 501 | 48.14 |
| 1.839 | 15 | 432 | 49.54 |
| 1.800 | 4 | 352 | 50.66 |
| 1.798 | 2 | 243 | 50.74 |
| 1.779 | 4 | 053 | 51.33 |
| 1.742 | 7 | 014 | 52.49 |
| 1.7327 | 13 | 442 | 52.79 |
| 1.6585 | 4 | 081 | 55.35 |
| 1.6541 | 3 | 204 | 55.51 |
| 1.6193 | 6 | 452 | 56.81 |

# Ammonium strontium chromium oxide, $(NH_4)_2Sr(CrO_4)_2$

Sample
The sample was precipitated by adding a strong solution of $SrCl_2$ to one of $(NH_4)_2CrO_4$, following the method of Schwarz [1966]. This material gave somewhat broad peaks which suggest that the compound may be of lower symmetry.

Color
Dark orange yellow

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many other double chromates and sulfates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.758(1) Å
c = 22.027(4)

Volume
632.3 $Å^3$

Density
(calculated) 2.802 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 2.2(3)

Additional pattern
1. PDF card 19-70 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 345, 230.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.345 | 60 | 003 | 12.04 |
| 4.868 | 5 | 101 | 18.21 |
| 4.546 | 45 | 012 | 19.51 |
| 3.696 | 10 | 104 | 24.06 |
| 3.672 | 6 | 006 | 24.22 |
| 3.300 | 100 | 015 | 27.00 |
| 2.881 | 60 | 110 | 31.02 |
| 2.680 | 30 | 113 | 33.41 |
| 2.662 | 13 | 107 | 33.64 |
| 2.434 | 4 | 202 | 36.90 |
| 2.411 | 2 | 018 | 37.26 |
| 2.271 | 8 | 024 | 39.65 |
| 2.266 | 9 | 116 | 39.75 |
| 2.169 | 20 | 205 | 41.61 |
| 2.015 | 20 | 1·0·10 | 44.95 |
| 1.955 | 2 | 027 | 46.42 |
| 1.857 | 6 | 0·1·11,122 | 49.01 |
| 1.848 | 11 | 208 | 49.26 |
| 1.836 | 6 | 0·0·12 | 49.61 |
| 1.783 | 2 | 214 | 51.19 |
| 1.732 | 11 | 125 | 52.81 |
| 1.662 | 6 | 300 | 55.23 |
| 1.651 | 5 | 0·2·10 | 55.63 |
| 1.619 | 4 | 303,217 | 56.81 |
| 1.604 | 3 | 1·0·13 | 57.40 |
| 1.554 | 2 | 128 | 59.41 |
| 1.5481 | 2 | 1·1·12 | 59.68 |
| 1.4682 | 3 | 0·0·15 | 63.29 |
| 1.4392 | 5 | 220 | 64.72 |
| 1.4319 | 11 | 2·1·10 | 65.09 |

# Barium vanadium oxide, $Ba_3(VO_4)_2$

Sample
Prepared by heating stoichiometric amounts of $BaCO_3$ and $V_2O_5$ at 825 °C, regrinding and reheating at 860 °C for 1½ hours, grinding again and heating on Méker burner (~1100 °C) for 10 minutes to improve crystallization.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$. The structure was determined by Zachariasen [1948] and refined by Süsse and Buerger [1970].

NBS lattice constants of this sample:

a = 5.7845(2) Å
c = 21.317(1)

Volume
617.73 $Å^3$

Density
(calculated) 5.176 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 4.7(4)

Additional patterns
1. PDF card 19-144 [Lubin & Rittershaus, Gen'l. Tel. and Electronics, N.Y. (1966)].
2. PDF card 25-1192 [Smith et al., 1974].
3. Zachariasen [1948].

References

Smith, D. K., et al., (1974). Annual Report to the Joint Committee on Powder Diffraction Standards.

Süsse, P., and Buerger, M. J., (1970). Z. Kristallogr. 131, 161.

Zachariasen, W. H., (1948). Acta Crystallogr. 1, 263.


CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.09 | 4 | 003 | 12.47 |
| 4.878 | 11 | 101 | 18.17 |
| 4.537 | 3 | 012 | 19.55 |
| 3.651 | 12 | 104 | 24.36 |
| 3.247 | 100 | 015 | 27.45 |
| 2.893 | 75 | 110 | 30.88 |
| 2.487 | 4 | 021 | 36.09 |
| 2.439 | 7 | 202 | 36.82 |
| 2.369 | 9 | 009 | 37.95 |
| 2.353 | 3 | 018 | 38.22 |
| 2.267 | 11 | 024 | 39.72 |
| 2.243 | 6 | 116 | 40.17 |
| 2.160 | 40 | 205 | 41.79 |
| 1.962 | 25 | 1·0·10 | 46.24 |
| 1.934 | 4 | 027 | 46.95 |
| 1.886 | 3 | 211 | 48.20 |
| 1.833 | 10 | 119 | 49.71 |
| 1.785 | 3 | 214 | 51.14 |
| 1.731 | 25 | 125 | 52.85 |
| 1.670 | 13 | 300 | 54.92 |
| 1.624 | 12 | 0·2·10 | 56.64 |
| 1.543 | 1 | 128 | 59.90 |
| 1.511 | 2 | 306 | 61.30 |
| 1.457 | 4 | 0·1·14 | 63.85 |
| 1.446 | 10 | 220 | 64.38 |
| 1.421 | 4 | 0·0·15 | 65.66 |
| 1.416 | 13 | 2·1·10 | 65.92 |
| 1.386 | 1 | 131 | 67.53 |
| 1.3647 | 3 | 309 | 68.73 |
| 1.3445 | 1 | 134 | 69.91 |
| 1.3208 | 9 | 315 | 71.35 |
| 1.3010 | 2 | 2·0·14 | 72.61 |
| 1.2755 | 10 | 1·1·15 | 74.30 |
| 1.2438 | 1 | 042 | 76.53 |
| 1.2343 | 4 | 229 | 77.23 |
| 1.2324 | 2 | 318 | 77.37 |
| 1.2015 | 4 | 045 | 79.75 |
| 1.1864 | 3 | 1·2·14 | 80.97 |
| 1.1641 | 5 | 1·3·10 | 82.86 |
| 1.1235 | 1 | 324 | 86.57 |
| 1.1096 | 5 | 235 | 87.93 |
| 1.0947 | 4 | 1·0·19 | 89.44 |
| 1.0933 | 5 | 410 | 89.59 |
| 1.0824 | 6 | 3·0·15 | 90.74 |
| 1.0799 | 5 | 4·0·10 | 91.01 |
| 1.0425 | 3 | 0·1·20 | 95.27 |
| 1.0264 | 2 | 3·1·14 | 97.27 |
| 1.0239 | 2 | 0·2·19 | 97.57 |
| 1.0135 | 5 | 2·2·15 | 98.93 |
| 1.0114 | 7 | 3·2·10 | 99.22 |

| $CuK\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C<br>Internal standard W, a = 3.16524 Å | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) |
| 0.9927 | 2 | 419 | 101.78 |
| .9809 | 2 | 2•0•20 | 103.49 |
| .9753 | 2 | 505 | 104.34 |
| .9653 | 4 | 2•1•19 | 105.87 |
| .9641 | 4 | 330 | 106.06 |
| .9288 | 4 | 1•2•20 | 112.07 |
| .9242 | 3 | 425 | 112.91 |
| .9174 | 2 | 2•3•14 | 114.21 |
| .9067 | 2 | 0•5•10 | 116.32 |
| .8802 | 2 | 155 | 122.12 |
| .8729 | 1 | 1•3•19 | 123.87 |
| .8665 | 1 | 4•1•15 | 125.50 |

# Calcium iodate (lautarite), $Ca(IO_3)_2$

Sample
The preparation was begun by adding an aqueous solution of $Ca(NO_3)_2$ to one of $HIO_3$ to precipitate $Ca(IO_3)_2 \cdot 6H_2O$ which was then heated at 160°C. for six hours. It was heated again in a sealed glass tube at 240°C for several hours.

Color
Colorless

Structure
Monoclinic, $P2_1/n(14)$, Z=4, distorted perovskite type. [Gossner and Mussgnug, 1930]. The structure was determined by Gossner, [1937].

NBS lattice constants of this sample:

a = 7.280(1) Å
b = 11.304(2)
c = 7.148(1)
β = 106.36(2)°

Volume
564.4 $Å^3$

Density
(calculated) 4.588 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 2.45(4)

Additional Patterns
1. PDF card 1-386, labeled $Ca(IO_3)_2$ but data is for $Ca(IO_3)_2 \cdot H_2O$, brüggenite.

References
Gossner, B., (1937). Z. Krist. 96, 381.
Gossner, B., and Mussgnug, F., (1930). Z. Krist. 75, 410.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.93 | 12 | 110 | 14.93 |
| 5.866 | 5 | 011 | 15.09 |
| 5.779 | 5 | $\bar{1}01$ | 15.32 |
| 5.651 | 3 | 020 | 15.67 |
| 5.139 | 5 | $\bar{1}11$ | 17.24 |
| 4.360 | 50 | 021 | 20.35 |
| 4.037 | 17 | $\bar{1}21$,111 | 22.00 |
| 3.493 | 65 | 200 | 25.48 |
| 3.428 | 85 | 002 | 25.97 |
| 3.378 | 14 | $\bar{2}11$ | 26.36 |
| 3.336 | 40 | 210,$\bar{1}12$ | 26.70 |
| 3.318 | 30 | $\bar{1}30$ | 26.85 |
| 3.156 | 100 | $\bar{1}31$ | 28.25 |
| 3.001 | 18 | $\bar{2}21$ | 29.75 |
| 2.931 | 3 | 022 | 30.47 |
| 2.885 | 20 | $\bar{2}02$ | 30.97 |
| 2.840 | 35 | $\bar{1}31$ | 31.48 |
| 2.795 | 13 | $\bar{2}12$ | 31.99 |
| 2.726 | 10 | 211 | 32.83 |
| 2.703 | 4 | 112 | 33.12 |
| 2.619 | 2 | $\bar{1}40$ | 34.21 |
| 2.582 | 2 | $\bar{2}31$ | 34.71 |
| 2.560 | 6 | 230,$\bar{1}32$ | 35.02 |
| 2.515 | 8 | $\bar{2}21$ | 35.67 |
| 2.328 | 2 | $\bar{1}13$ | 38.65 |
| 2.292 | 5 | $\bar{2}32$ | 39.27 |
| 2.252 | 2 | 231 | 40.01 |
| 2.240 | 2 | 013,132 | 40.22 |
| 2.227 | 8 | $\bar{3}21$ | 40.48 |
| 2.199 | 5 | $\bar{3}12$ | 41.01 |
| 2.194 | 5 | $\bar{1}23$ | 41.11 |
| 2.161 | 18 | 202 | 41.77 |
| 2.151 | 8 | 150 | 41.97 |
| 2.146 | 5 | 051 | 42.06 |
| 2.122 | 5 | 212 | 42.57 |
| 2.120 | 5 | 023 | 42.64 |
| 2.067 | 3 | $\bar{2}23$ | 43.77 |
| 2.038 | 20 | $\bar{3}31$,301 | 44.42 |
| 2.012 | 30 | $\bar{1}33$,103 | 45.02 |
| 1.987 | 4 | 330,113 | 45.75 |
| 1.926 | 4 | $\bar{3}03$ | 47.16 |
| 1.917 | 6 | $\bar{3}21$ | 47.39 |
| 1.897 | 9 | $\bar{1}52$,$\bar{3}13$ | 47.91 |
| 1.884 | 9 | 060 | 48.27 |
| 1.840 | 3 | $\bar{3}41$ | 49.51 |
| 1.817 | 12 | 061 | 50.17 |
| 1.797 | 12 | 340 | 50.77 |
| 1.793 | 14 | 331 | 50.90 |
| 1.775 | 15 | 133 | 51.44 |
| 1.756 | 12 | $\bar{3}42$,152 | 52.05 |
| 1.7500 | 11 | $\bar{4}12$ | 52.23 |
| 1.7460 | 11 | $\bar{2}43$,$\bar{2}04$ | 52.36 |
| 1.7255 | 11 | 410,$\bar{2}14$ | 53.03 |
| 1.7138 | 14 | $\bar{3}33$ | 53.42 |
| 1.6863 | 4 | 213 | 54.36 |
| 1.6629 | 7 | $\bar{2}61$ | 55.19 |
| 1.6582 | 8 | 260,$\bar{1}62$ | 55.36 |
| 1.6514 | 6 | 062 | 55.61 |
| 1.6078 | 1 | 053 | 57.25 |
| 1.5911 | 4 | $\bar{3}52$,$\bar{3}43$ | 57.91 |
| 1.5836 | 4 | $\bar{2}53$,$\bar{2}34$ | 58.21 |
| 1.5780 | 5 | $\bar{2}62$ | 58.44 |
| 1.5735 | 5 | 170,411 | 58.62 |
| 1.5645 | 4 | 261 | 58.99 |
| 1.5602 | 4 | 034,162 | 59.17 |
| 1.5293 | 1 | $\bar{4}41$,421 | 60.49 |

# Calcium iodate hydrate, $Ca(IO_3)_2 \cdot 6H_2O$

Sample
The sample was prepared by adding an aqueous solution of $Ca(NO_3)_2$ to one of $HIO_3$. The loss in weight at 160°C indicated that it was a hexahydrate.

Color
Colorless

Optical Data
Biaxial, $N_\alpha$=1.604, $N_\beta$=1.644, $N_\gamma$=1.686, 2V is large. [Winchell and Winchell, 1964].

Structure
Orthorhombic, Fdd2 (43) from precession patterns [Perloff, 1976]. Z=6 (from agreement of experimental and calculated densities).

NBS lattice constants of this sample

a = 14.866(3)Å
b = 23.015(5)
c = 6.392(1)

Volume
2187.1Å$^3$

Density
(calculated) 2.268 g/cm$^2$

Reference Intensity
$I/I_{corundum}$ = 2.4(3)

References
Perloff, A. (1976). Private communication.
Winchell, A. N., and Winchell, H. (1964). The Microscopical Characters of Artificial Inorganic Solid Substances (Academic Press, New York and London) p. 109.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.75 | 50 | 040 | 15.39 |
| 5.69 | 60 | 111 | 15.55 |
| 4.65 | 100 | 131 | 19.04 |
| 3.86 | 25 | 311 | 23.02 |
| 3.714 | 40 | 400 | 23.94 |
| 3.625 | 11 | 151 | 24.54 |
| 3.538 | 5 | 420 | 25.14 |
| 3.489 | 55 | 331 | 25.51 |
| 3.406 | 20 | 260 | 26.14 |
| 3.121 | 40 | 440 | 28.58 |
| 3.078 | 6 | 022 | 28.99 |
| 2.983 | 5 | 351 | 29.93 |
| 2.936 | 40 | 202 | 30.42 |
| 2.878 | 25 | 080 | 31.05 |
| 2.867 | 30 | 171 | 31.17 |
| 2.842 | 8 | 222 | 31.45 |
| 2.676 | 19 | 511 | 33.46 |
| 2.669 | 15 | 460 | 33.55 |
| 2.616 | 55 | 242 | 34.25 |
| 2.544 | 13 | 531 | 35.25 |
| 2.517 | 16 | 371 | 35.64 |
| 2.455 | 3 | 062 | 36.57 |
| 2.370 | 3 | 422 | 37.93 |
| 2.343 | 18 | 191 | 38.39 |
| 2.331 | 6 | 262 | 38.60 |
| 2.275 | 8 | 640,480 | 39.59 |
| 2.234 | 1 | 442 | 40.34 |
| 2.198 | 7 | 2·10·0 | 41.03 |
| 2.142 | 3 | 391 | 42.15 |
| 2.101 | 15 | 113 | 43.02 |
| 2.081 | 9 | 660 | 43.43 |
| 2.055 | 11 | 282 | 44.03 |
| 2.048 | 8 | 462 | 44.18 |
| 2.034 | 12 | 133 | 44.51 |
| 2.007 | 5 | 711 | 45.14 |
| 1.971 | 11 | 1·11·1 | 46.02 |
| 1.956 | 7 | 4·10·0 | 46.38 |
| 1.951 | 19 | 313,731 | 46.52 |
| 1.930 | 6 | 622 | 47.05 |
| 1.917 | 1 | 0·12·0,153 | 47.39 |
| 1.896 | 4 | 333 | 47.95 |
| 1.868 | 9 | 0·10·2 | 48.71 |
| 1.853 | 25 | 642,482 | 49.12 |
| 1.846 | 20 | 751,3·11·1 | 49.33 |
| 1.802 | 2 | 353 | 50.62 |
| 1.775 | 11 | 173 | 51.43 |
| 1.744 | 4 | 662 | 52.42 |
| 1.728 | 4 | 513 | 52.96 |
| 1.719 | 3 | 771 | 53.25 |
| 1.690 | 6 | 533 | 54.25 |
| 1.683 | 8 | 373 | 54.49 |
| 1.669 | 7 | 4·10·2 | 54.96 |
| 1.653 | 6 | 5·11·1 | 55.55 |
| 1.606 | 8 | 2·12·2,2·14·0 | 57.34 |
| 1.599 | 4 | 004 | 57.61 |
| 1.566 | 2 | 931 | 58.95 |
| 1.562 | 3 | 880 | 59.11 |
| 1.549 | 3 | 224 | 59.65 |
| 1.532 | 6 | 573 | 60.37 |

# Cesium iron chloride hydrate, $Cs_2FeCl_5 \cdot H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of a 2:1 molar aqueous solution of CsCl and $FeCl_3$.

Color
Deep reddish orange.

Structure
Orthorhombic, Amam(63), Z=4. Perloff [1976] by single crystal study found that $Cs_2FeCl_5 \cdot H_2O$ was isostructural with $Cs_2RuCl_5 \cdot H_2O$. The structure of $Cs_2RuCl_5 \cdot H_2O$ had been determined by Hopkins et al. [1966].

NBS lattice constants of this sample:

a = 8.070(1)Å
b = 17.326(2)
c = 7.436(1)

Volume
1039.8 $Å^3$

Density
(calculated) 3.302 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 1.9(2)

References
Hopkins, T. E., Zalkin, A., Templeton, D. H., and Adamson, M. G. (1966). Inorg. Chem. 5, 1431.
Perloff, A. (1976). Private communication.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.83 | 8 | 011 | 12.95 |
| 5.91 | 7 | 120 | 14.97 |
| 5.21 | 4 | 111 | 17.00 |
| 4.565 | 40 | 031 | 19.43 |
| 4.335 | 6 | 040 | 20.47 |
| 4.037 | 45 | 200 | 22.00 |
| 3.973 | 100 | 131 | 22.36 |
| 3.816 | 5 | 140 | 23.29 |
| 3.719 | 25 | 002 | 23.91 |
| 3.660 | 4 | 220 | 24.30 |
| 3.476 | 12 | 211 | 25.61 |
| 3.418 | 3 | 022 | 26.05 |
| 3.143 | 10 | 122,051 | 28.37 |
| 3.024 | 20 | 231 | 29.52 |
| 2.950 | 75 | 240 | 30.27 |
| 2.888 | 8 | 060 | 30.94 |
| 2.822 | 55 | 042 | 31.68 |
| 2.736 | 95 | 202 | 32.71 |
| 2.721 | 45 | 160 | 32.89 |
| 2.665 | 5 | 142 | 33.60 |
| 2.571 | 4 | 320 | 34.87 |
| 2.502 | 2 | 311 | 35.86 |
| 2.479 | 4 | 251 | 36.20 |
| 2.454 | 4 | 013 | 36.59 |
| 2.349 | 2 | 071,260+ | 38.29 |
| 2.318 | 20 | 331 | 38.82 |
| 2.286 | 4 | 340 | 39.39 |
| 2.280 | 5 | 062 | 39.49 |
| 2.255 | 11 | 171 | 39.95 |
| 2.194 | 25 | 162 | 41.10 |
| 2.165 | 13 | 080 | 41.68 |
| 2.113 | 4 | 322 | 42.76 |
| 2.093 | 3 | 180 | 43.20 |
| 2.018 | 12 | 400,053 | 44.89 |
| 1.984 | 12 | 233 | 45.70 |
| 1.968 | 4 | 360 | 46.08 |
| 1.934 | 2 | 411 | 46.94 |
| 1.908 | 4 | 280 | 47.62 |
| 1.872 | 4 | 082 | 48.60 |
| 1.859 | 11 | 004 | 48.97 |
| 1.845 | 6 | 431 | 49.36 |
| 1.829 | 3 | 440 | 49.82 |
| 1.823 | 3 | 182 | 49.99 |
| 1.804 | 4 | 253 | 50.56 |
| 1.773 | 8 | 402,124 | 51.51 |
| 1.770 | 10 | 371 | 51.61 |
| 1.739 | 18 | 362,333 | 52.59 |
| 1.711 | 6 | 173 | 53.51 |
| 1.697 | 16 | 282,451 | 53.98 |
| 1.693 | 12 | 1•10•0 | 54.12 |
| 1.654 | 2 | 460 | 55.53 |
| 1.640 | 8 | 442 | 56.00 |
| 1.591 | 4 | 2•10•0 | 57.90 |
| 1.587 | 4 | 520 | 58.06 |
| 1.573 | 8 | 244 | 58.65 |
| 1.570 | 9 | 511,0•10•2 | 58.75 |
| 1.535 | 6 | 164 | 60.25 |
| 1.533 | 5 | 391 | 60.34 |
| 1.5207 | 6 | 093 | 60.87 |
| 1.5126 | 6 | 540 | 61.23 |
| 1.5101 | 6 | 433 | 61.34 |
| 1.4757 | 4 | 480 | 62.93 |
| 1.4565 | 3 | 3•10•0 | 63.86 |
| 1.4088 | 6 | 560 | 66.29 |

# Copper phosphate, $Cu(PO_3)_2$

Sample
The sample was made by heating $CuCO_3$ and $H_3PO_4$ together at 760 °C for 45 minutes.

Color
Very pale green

Structure
Monoclinic, I2/a (15) or Ia (9), Z = 8, [Beucher and Grenier, 1968]. Those authors gave the cell in the settings C2/c (15) or Cc (9).

NBS lattice constants of this sample:

a = 11.584(2) Å
b = 8.081(2)
c = 9.569(2)
β = 107.91(2)°

Volume
852.3 $Å^3$

Density
(calculated) 3.452 $g/cm^3$

Reference Intensity
$I/I_{corundum}$ = 1.4

Additional patterns
1. PDF card 21-998 [Ball, 1968]
2. PDF card 25-1196 [Smith et al., 1974]

References

Ball, M. C., (1968). J. Chem. Soc. (London) 5A, 1113.
Beucher, M., and Grenier, J-C., (1968). Mater. Res. Bull. 3, 643.
Smith, D. K., et al., Annual Report to the Joint Committee on Powder Diffraction Standards, 1974.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.52 | 7 | 110 | 13.56 |
| 6.046 | 55 | 011 | 14.64 |
| 5.507 | 5 | 200 | 16.08 |
| 4.565 | 20 | $\bar{2}11$ | 19.43 |
| 4.205 | 4 | $\bar{2}02$ | 21.11 |
| 4.101 | 35 | $\bar{1}12$ | 21.65 |
| 3.716 | 30 | $2\bar{1}1$ | 23.93 |
| 3.645 | 10 | $\bar{1}21$ | 24.40 |
| 3.448 | 40 | 112 | 25.82 |
| 3.376 | 17 | 121 | 26.38 |
| 3.343 | 50 | 310 | 26.64 |
| 3.259 | 10 | $\bar{2}20$ | 27.34 |
| 2.912 | 100 | $\bar{2}22$ | 30.68 |
| 2.841 | 30 | 013 | 31.46 |
| 2.783 | 8 | $\bar{3}21$ | 32.14 |
| 2.756 | 35 | 400 | 32.46 |
| 2.727 | 12 | $\bar{4}11$ | 32.82 |
| 2.617 | 2 | 130 | 34.23 |
| 2.447 | 25 | $\bar{2}22$ | 36.69 |
| 2.423 | 6 | $\bar{2}31$ | 37.08 |
| 2.334 | 17 | $\bar{4}11$ | 38.55 |
| 2.301 | 8 | $\bar{3}23$ | 39.11 |
| 2.277 | 7 | 420,004 | 39.55 |
| 2.190 | 8 | $\bar{3}14$ | 41.19 |
| 2.127 | 4 | 510 | 42.47 |
| 2.101 | 6 | $\bar{4}04$ | 43.02 |
| 2.089 | 10 | $\bar{4}02$ | 43.28 |
| 2.049 | 6 | $\bar{2}24$ | 44.17 |
| 2.030 | 25 | $\bar{2}33$ | 44.59 |
| 2.007 | 4 | $\bar{5}21$ | 45.14 |
| 1.877 | 5 | $\bar{5}23$ | 48.46 |
| 1.861 | 6 | $\bar{2}15$ | 48.89 |
| 1.835 | 4 | $\bar{3}32$ | 49.63 |
| 1.821 | 4 | $\bar{2}42$ | 50.05 |
| 1.779 | 7 | 233 | 51.32 |
| 1.738 | 25 | $512,\bar{3}34$ + | 52.61 |
| 1.735 | 16 | $\bar{6}22$ | 52.73 |
| 1.709 | 6 | $\bar{6}04$ | 53.59 |
| 1.6724 | 5 | 620 | 54.85 |
| 1.6663 | 4 | 611 | 55.07 |
| 1.6378 | 6 | $\bar{3}43$ | 56.11 |
| 1.6293 | 8 | 440 | 56.43 |
| 1.5906 | 8 | 051 | 57.93 |
| 1.5743 | 6 | $\bar{6}24$ | 58.59 |
| 1.5600 | 13 | $\bar{2}35,215$ | 59.18 |
| 1.5450 | 5 | $710,\bar{4}06$ | 59.81 |
| 1.5411 | 4 | $\bar{1}16$ | 59.98 |
| 1.5385 | 4 | 404 | 60.09 |
| 1.5204 | 9 | $\bar{5}41,\bar{6}33$ | 60.88 |
| 1.5106 | 12 | 044 | 61.32 |
| 1.4932 | 3 | $\bar{4}35$ | 62.11 |
| 1.4876 | 7 | 433,152 | 62.37 |
| 1.4827 | 5 | $\bar{2}26$ | 62.60 |
| 1.4563 | 9 | $\bar{5}16,444$ | 63.87 |

# Lead chromium oxide, $Pb_2CrO_5$

Sample
The sample was prepared by T. Negas by heating PbO (massicot) and $Cr_2O_3$ together at 630-650 °C for 92 hours followed by regrinding and heating.

Color
Deep orange.

Structure
Monoclinic I2/m (12), Z = 4, isostructural with $Pb_2SO_5$. The structure has been studied by Ruckman et al. [1972]. These authors gave the cell in a setting in C2/m (12).

NBS lattice constants of this sample:

a = 12.728(1) Å
b = 5.6782(5)
c = 7.1414(6)
β = 95.23(1)°

Volume
513.96 $Å^3$

Density
(calculated) 7.061 $g/cm^3$

Reference Intensity
$I/I_{corundum}$ = 5.1(3)

Additional patterns
1. PDF card 26-832 [Ruckman et al., 1972].
2. Negas [1968].

References
Negas, T., (1968). J. Am. Ceram. Soc. 51, 716.
Ruckman, J. C., Morrison, R. T. W., and Buck, R. H. (1972). J. Chem. Soc. Dalton Trans. 1972, 426.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.46 | 16 | $\bar{1}01$ | 13.69 |
| 6.34 | 16 | 200 | 13.95 |
| 5.973 | 12 | 101 | 14.82 |
| 5.184 | 2 | 110 | 17.09 |
| 4.438 | 13 | 011 | 19.99 |
| 3.786 | 9 | $\bar{3}01$ | 23.48 |
| 3.737 | 4 | $\bar{2}11$ | 23.79 |
| 3.555 | 3 | 002 | 25.03 |
| 3.542 | 6 | 211 | 25.12 |
| 3.390 | 100 | 310 | 26.27 |
| 3.230 | 15 | $\bar{2}02$ | 27.59 |
| 3.169 | 1 | 400 | 28.14 |
| 2.984 | 80 | 202,$\bar{1}12$ | 29.92 |
| 2.881 | 20 | 112 | 31.02 |
| 2.838 | 35 | 020 | 31.50 |
| 2.651 | 4 | $\bar{4}11$ | 33.78 |
| 2.601 | 2 | $\bar{1}21$ | 34.46 |
| 2.592 | 4 | 220 | 34.58 |
| 2.564 | 6 | 121 | 34.96 |
| 2.512 | 15 | 411 | 35.72 |
| 2.480 | 16 | $\bar{4}02$ | 36.19 |
| 2.460 | 8 | $\bar{5}01$ | 36.49 |
| 2.368 | 8 | $\bar{1}03$,312 | 37.96 |
| 2.314 | 12 | 510 | 38.88 |
| 2.272 | 13 | $\bar{3}21$ | 39.64 |
| 2.266 | 16 | 402 | 39.75 |
| 2.204 | 2 | 321 | 40.92 |
| 2.188 | 5 | 013 | 41.23 |
| 2.132 | 6 | $\bar{2}22$ | 42.36 |
| 2.113 | 10 | 600 | 42.77 |
| 2.058 | 20 | 222 | 43.97 |
| 2.018 | 2 | $\bar{5}12$ | 44.88 |
| 1.992 | 5 | 303 | 45.50 |
| 1.951 | 4 | $\bar{6}11$ | 46.51 |
| 1.875 | 9 | $\bar{4}13$ | 48.50 |
| 1.869 | 19 | 512,$\bar{4}22$ | 48.68 |
| 1.860 | 8 | $\bar{5}21$ | 48.94 |
| 1.830 | 2 | 031 | 49.80 |
| 1.820 | 2 | $\bar{1}23$ | 50.09 |
| 1.7972 | 1 | 521 | 50.76 |
| 1.7779 | 9 | 004 | 51.35 |
| 1.7708 | 11 | $\bar{4}22$ | 51.57 |
| 1.7541 | 5 | $\bar{2}04$ | 52.10 |
| 1.7469 | 1 | 602,231 | 52.33 |
| 1.7273 | 11 | 330 | 52.97 |
| 1.7177 | 5 | 701 | 53.29 |
| 1.6947 | 7 | $\bar{6}20$ | 54.07 |
| 1.6654 | 11 | $\bar{1}32$ | 55.10 |
| 1.6627 | 4 | 114 | 55.20 |
| 1.6473 | 3 | 132 | 55.76 |

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.6304 | 5 | $\bar{3}23$ | 56.39 |
| 1.6240 | 4 | $\bar{3}14$ | 56.63 |
| 1.6076 | 8 | $\bar{7}12$ | 57.26 |
| 1.5876 | 1 | $\bar{6}13$ | 58.05 |
| 1.5841 | 2 | 800 | 58.19 |
| 1.5753 | 2 | $\bar{6}22$ | 58.55 |
| 1.5682 | 3 | 431 | 58.84 |
| 1.5291 | 10 | $\bar{5}23$,314 | 60.50 |
| 1.5197 | 8 | $\bar{8}11$ | 60.91 |
| 1.5068 | 9 | 024,$\bar{7}03$ | 61.49 |
| 1.5020 | 4 | 712 | 61.71 |
| 1.4919 | 4 | $\bar{2}24$ | 62.17 |
| 1.4789 | 2 | 033 | 62.78 |
| 1.4699 | 10 | $\bar{5}14$,721 | 63.21 |
| 1.4593 | 4 | 613,$\bar{2}33$ | 63.72 |
| 1.4313 | 2 | $\bar{5}23$ | 65.12 |
| 1.4260 | 2 | $\bar{6}04$ | 65.39 |
| 1.4195 | 5 | 040 | 65.73 |
| 1.3991 | 2 | 105,$\bar{6}31$ | 66.81 |

# Lead hydrogen arsenate (schultenite), $PbHAsO_4$

Sample
The sample was precipitated by adding a concentrated aqueous solution of $Pb(NO_3)_2$ to one of $As_2O_5$.

Color
Colorless

Optical data
Biaxial (+), $N_\alpha$ = 1.890, $N_\beta$ = 1.910, $N_\gamma$ = 1.976, 2V is medium.

Structure
Monoclinic, P2/a (13), Z = 2. [Claringbull, 1950].

NBS lattice constants of this sample:

a = 5.8421(6) Å
b = 6.7545(6)
c = 4.8575(6)
β = 95.40(1)°

Volume
190.83 $Å^3$

Density
(calculated) 6.041 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 7.6(2)

Additional patterns
1. PDF card 11-141 [Claringbull, 1950]
2. Hanawalt et al., [1938]

References

Claringbull, G. F., (1950). Mineral. Mag. 29, 287.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.


CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.74 | 25 | 010 | 13.12 |
| 4.833 | 12 | 001 | 18.34 |
| 4.410 | 18 | 110 | 20.12 |
| 3.931 | 4 | 011 | 22.60 |
| 3.376 | 100 | $\bar{1}11$,020 | 26.38 |
| 3.149 | 70 | 111 | 28.32 |
| 2.919 | 13 | 120 | 30.60 |
| 2.909 | 25 | 200 | 30.71 |
| 2.769 | 6 | 021 | 32.30 |
| 2.671 | 5 | 210 | 33.52 |
| 2.603 | 4 | $\bar{2}01$ | 34.43 |
| 2.555 | 16 | $\bar{1}21$ | 35.10 |
| 2.450 | 5 | 121 | 36.65 |
| 2.419 | 11 | 002 | 37.14 |
| 2.395 | 5 | 201 | 37.53 |
| 2.276 | 1 | 012 | 39.56 |
| 2.252 | 6 | 030 | 40.00 |
| 2.204 | 16 | $\bar{2}20$ | 40.92 |
| 2.187 | 7 | $\bar{1}12$ | 41.24 |
| 2.100 | 3 | 130 | 43.04 |
| 2.061 | 6 | $\bar{2}21$ | 43.89 |
| 2.041 | 3 | 031 | 44.34 |
| 1.967 | 11 | $\bar{0}22$ | 46.12 |
| 1.951 | 12 | $\bar{2}02$,$\bar{1}31$ | 46.51 |
| 1.9024 | 6 | 131 | 47.77 |
| 1.8751 | 2 | $\bar{2}12$ | 48.51 |
| 1.8636 | 4 | 310 | 48.83 |
| 1.8203 | 2 | $\bar{1}22$ | 50.07 |
| 1.7939 | 10 | $\bar{3}11$ | 50.86 |
| 1.7802 | 14 | 230 | 51.28 |
| 1.7200 | 1 | $\bar{2}12$ | 53.21 |
| 1.7029 | 1 | $\bar{2}31$ | 53.79 |
| 1.6886 | 11 | 040,311 + | 54.28 |
| 1.6820 | 6 | 320 | 54.51 |
| 1.6484 | 5 | 032 | 55.72 |
| 1.6410 | 2 | $\bar{2}31$ | 55.99 |
| 1.6298 | 3 | $\bar{3}21$ | 56.41 |
| 1.6217 | 2 | $\bar{1}40$ | 56.72 |
| 1.6123 | 2 | $\bar{1}32$,003 | 57.08 |
| 1.5939 | < 1 | 041 | 57.80 |
| 1.5740 | 5 | 222 | 58.60 |
| 1.5590 | 3 | $\bar{1}32$ | 59.22 |
| 1.5497 | 10 | $\bar{1}41$,321 + | 59.61 |
| 1.5254 | 5 | 141 | 60.66 |
| 1.4806 | 5 | 113 | 62.70 |
| 1.4749 | 5 | $\bar{2}32$ | 62.97 |
| 1.4606 | 2 | 240 | 63.66 |
| 1.4542 | 3 | 023,400 | 63.97 |
| 1.4404 | 2 | $\bar{1}23$ | 64.66 |
| 1.4346 | 2 | $\bar{3}31$ | 64.95 |
| 1.4157 | 1 | 312 | 65.93 |
| 1.3954 | 2 | 232 | 67.01 |
| 1.3842 | 2 | 042,123 | 67.63 |
| 1.3788 | 2 | $\bar{3}31$ | 67.93 |
| 1.3634 | < 1 | $\bar{1}42$ | 68.80 |
| 1.3507 | 2 | 050 | 69.54 |
| 1.3353 | 2 | $\bar{4}20$ | 70.46 |
| 1.3167 | 1 | $\bar{4}21$ | 71.61 |
| 1.3102 | < 1 | $\bar{0}33$ | 72.02 |
| 1.3010 | 3 | $\bar{4}02$,051 | 72.61 |
| 1.2774 | 3 | $\bar{4}12$,$\bar{3}13$ + | 74.17 |
| 1.2592 | 1 | 421,223 | 75.43 |
| 1.2503 | 2 | $\bar{3}41$ | 76.06 |
| 1.2251 | 3 | 250,242 | 77.92 |
| 1.2132 | 4 | 341 | 78.83 |
| 1.1990 | 2 | $\bar{2}51$ | 79.95 |
| 1.1972 | 1 | 402 | 80.09 |
| 1.1791 | 2 | 052,412 | 81.58 |
| 1.1766 | 2 | 251 | 81.79 |
| 1.1679 | 2 | 313 | 82.53 |
| 1.1586 | 2 | $\bar{1}43$ | 83.34 |
| 1.1564 | 2 | $\bar{3}42$ | 83.54 |

# Lithium silicate, $Li_2SiO_3$

Sample
The sample was prepared by heating a 1:1 molar mixture of $Li_2CO_3$ and dried silica gel at 860 °C for 5 minutes; the material was ground and reheated for 5 minutes at 860 °C. A final heating for several minutes at about 1200 °C followed.

Color
Colorless

Structure
Orthorhombic, $Ccm2_1(36)$, Z = 4, [Seeman, 1956], isostructural with $Na_2SiO_3$, low $(Na,Li)SiO_3$ [West, 1976] and $Li_2GeO_3$ [Völlenkle and Wittman, 1968].

NBS lattice constants of this sample:

a = 5.3975(6) Å
b = 9.3974(6)
c = 4.6615(5)

Volume
236.44 $Å^3$

Density
(calculated) 2.527 $g/cm^3$

Additional patterns
1. PDF card 15-519 [Lam, Sheffield, England].
2. West [1976].

References
Seemann, H. (1956). Acta Crystallogr. 9, 251.
Völlenkle, H., and Wittmann, A. (1968). Monatsh. Chem. 99, 244.
West, A. R. (1976). J. Am. Ceram. Soc. 59, 118.

$CuK\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 4.69 | 100 | 020,110 | 18.91 |
| 3.301 | 65 | 111 | 26.99 |
| 2.708 | 65 | 130 | 33.05 |
| 2.700 | 45 | 200 | 33.15 |
| 2.342 | 19 | 131,220 | 38.41 |
| 2.331 | 20 | 002 | 38.60 |
| 2.091 | 7 | 221 | 43.24 |
| 2.085 | 5 | 022,112 | 43.36 |
| 1.7747 | 4 | 150 | 51.45 |
| 1.7667 | 9 | 310,132 | 51.70 |
| 1.7638 | 8 | 202 | 51.79 |
| 1.6563 | 7 | 241 | 55.43 |
| 1.6522 | 7 | 311,222 | 55.58 |
| 1.5665 | 12 | 060 | 58.91 |
| 1.5605 | 15 | 330 | 59.16 |
| 1.4747 | 3 | 113 | 62.98 |
| 1.4105 | 1 | 242 | 66.20 |
| 1.4079 | 1 | 312 | 66.34 |
| 1.3547 | 3 | 260 | 69.31 |
| 1.3475 | 5 | 133 | 69.73 |
| 1.3001 | 5 | 062,350 | 72.67 |
| 1.2965 | 8 | 332,401 + | 72.90 |
| 1.2544 | 3 | 171 | 75.77 |
| 1.2495 | 2 | 421 | 76.12 |
| 1.1747 | 2 | 080 | 81.95 |
| 1.1710 | 2 | 262 | 82.27 |
| 1.1681 | 2 | 243,402 | 82.52 |
| 1.1350 | 3 | 352,441 | 85.48 |
| 1.0770 | <1 | 280 | 91.32 |
| 1.0759 | <1 | 370 | 91.44 |
| 1.0700 | <1 | 204 | 92.09 |
| 1.0488 | 1 | 082 | 94.52 |
| 1.0452 | 1 | 511 | 94.95 |
| 1.0441 | <1 | 044 | 95.08 |
| 1.0253 | 1 | 190 | 97.40 |
| 1.0212 | 2 | 263 | 97.93 |
| 1.0188 | 1 | 403 | 98.24 |
| 1.0013 | 1 | 191 | 100.58 |
| 0.9984 | 2 | 461,173 | 100.98 |
| 0.9778 | <1 | 282 | 103.96 |
| 0.9769 | <1 | 372 | 104.10 |
| 0.9738 | 1 | 244 | 104.57 |
| 0.9727 | <1 | 314 | 104.73 |
| 0.9397 | <1 | 0·10·0 | 110.12 |
| 0.9384 | <1 | 192 | 110.34 |
| 0.9348 | 1 | 532,443 + | 110.98 |
| 0.9337 | 1 | 334 | 111.18 |

# Lithium tantalum oxide, $LiTaO_3$

Sample
The sample was prepared as a precipitate by adding LiOH to a solution of hydrolyzed $Ta_2O_5$. This was further crystallized by heating at 860°C overnight.

Color
Colorless

Structure
Hexagonal, R3c (161), Z=6, by analogy with $LiNbO_3$ which was studied by Bailey [1952].

NBS lattice constants of this sample:

a = 5.1530(4) Å
c = 13.755(2)

Volume
316.30 $Å^3$

Reference intensity
$I/I_{corundum}$ = 11.8(5)

Density
(calculated) 7.430 $g/cm^3$

Additional pattern
1. PDF card 9-187 [Lapickij and Simanov, 1955].

References
Bailey, P., thesis, Bristol (1952) quoted by Megaw, H. D. (1954). Acta Cryst. 7, 187.
Lapickij, A. V. and Simanov, J. P. (1955). Zh. Fiz. Khim. 29, 1201.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 3.745 | 100 | 012 | 23.74 |
| 2.723 | 40 | 104 | 32.86 |
| 2.577 | 25 | 110 | 34.79 |
| 2.292 | 4 | 006 | 39.28 |
| 2.245 | 3 | 113 | 40.13 |
| 2.122 | 14 | 202 | 42.57 |
| 1.871 | 16 | 024 | 48.62 |
| 1.712 | 20 | 116 | 53.48 |
| 1.638 | 14 | 122 | 56.12 |
| 1.604 | 6 | 018 | 57.41 |
| 1.5139 | 11 | 214 | 61.17 |
| 1.4874 | 6 | 300 | 62.38 |
| 1.3621 | 3 | 208 | 68.88 |
| 1.3145 | 3 | 119,1·0·10 | 71.75 |
| 1.2883 | 3 | 220 | 73.44 |
| 1.2481 | 3 | 306 | 76.22 |
| 1.2183 | 4 | 312 | 78.44 |
| 1.2043 | 4 | 128 | 79.53 |
| 1.1710 | 2 | 0·2·10 | 82.27 |
| 1.1648 | 4 | 134 | 82.80 |
| 1.1463 | 1 | 0·0·12 | 84.44 |
| 1.1231 | 3 | 226 | 86.61 |
| 1.10. 2 | 1 | 042 | 88.78 |
| 1.0664 | 2 | 2·1·10 | 92.50 |
| 1.0471 | 2 | 137,1·1·12 | 94.72 |
| 1.0126 | 2 | 232 | 99.06 |
| 1.0047 | 2 | 318,1·2·11 | 100.12 |
| 0.9812 | 2 | 324 | 103.45 |
| .9740 | 2 | 410 | 104.54 |

# Manganese phosphate, $Mn(PO_3)_2$

Sample
The sample was prepared by melting $MnCl_2$ with $H_3PO_4$ in molar proportions of 1:2.

Color
Pale pink

Structure
Monoclinic, I2/a (15) or Ia (9), Z = 8 [Beucher and Grenier, 1968]. Those authors gave the cell in the settings C2/c (15) or Cc (9).

NBS lattice constants of this sample

a = 11.359(2) Å
b = 8.472(2)
c = 10.176(2)
β = 112.06°(2)

Volume
907.57 $Å^3$

Density
(calculated) 3.116 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 0.89(11)

Additional pattern
1. PDF card 21-554 [Lee and Browne, 1968].

References
Beucher, M., and Grenier, J. C., (1968). Mater. Res. Bull. 3, 643.
Lee, J. D., and Browne, L. S., (1968). J. Chem. Soc. A 559.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.29 | 30 | 011 | 14.06 |
| 5.26 | 4 | 200 | 16.85 |
| 4.71 | 13 | 002 | 18.81 |
| 4.65 | 13 | $\bar{2}11$ | 19.07 |
| 4.348 | 35 | $\bar{1}12$ | 20.41 |
| 3.613 | 20 | 211 | 24.62 |
| 3.468 | 30 | 112 | 25.67 |
| 3.300 | 10 | 220 | 27.00 |
| 3.242 | 35 | $\bar{3}10$ | 27.49 |
| 3.065 | 100 | $\bar{2}22$ | 29.11 |
| 2.998 | 3 | 202 | 29.78 |
| 2.947 | 20 | 013 | 30.30 |
| 2.728 | 3 | $\bar{1}30$ | 32.80 |
| 2.681 | 4 | $\bar{4}11$ | 33.39 |
| 2.632 | 20 | 400 | 34.03 |
| 2.521 | 5 | $\bar{2}31$ | 35.59 |
| 2.446 | 20 | $\bar{2}22$ | 36.71 |
| 2.424 | 7 | $\bar{3}23$ | 37.06 |
| 2.358 | 3 | $\bar{0}04$ | 38.13 |
| 2.331 | 9 | $\bar{3}14,\bar{4}22$ | 38.59 |
| 2.236 | 11 | $\bar{4}11,420$ | 40.30 |
| 2.218 | 2 | $\bar{4}04$ | 40.64 |
| 2.200 | 2 | $\bar{3}30$ | 41.00 |
| 2.175 | 4 | $\bar{2}24$ | 41.48 |
| 2.145 | 19 | $\bar{2}33$ | 42.09 |
| 2.118 | 4 | 040 | 42.66 |
| 2.001 | 6 | $\bar{4}02$ | 45.29 |
| 1.979 | 5 | $\bar{2}15$ | 45.81 |
| 1.965 | 2 | $\bar{4}24,240$ | 46.16 |
| 1.928 | 3 | $\bar{5}23$ | 47.11 |
| 1.890 | 3 | $\bar{4}33$ | 48.10 |
| 1.864 | 4 | $\bar{4}15$ | 48.82 |
| 1.839 | 6 | $\bar{3}34$ | 49.54 |
| 1.802 | 7 | $\bar{1}25,233$ | 50.60 |
| 1.767 | 5 | $\bar{5}32$ | 51.70 |
| 1.735 | 4 | 224 | 52.71 |
| 1.728 | 11 | $242,\bar{6}22$ | 52.93 |
| 1.687 | 2 | $\bar{4}42$ | 54.35 |
| 1.667 | 10 | $051,\bar{5}12$ | 55.05 |
| 1.6503 | 12 | $440,\bar{4}06$ | 55.65 |

# Nickel phosphate, $Ni(PO_3)_2$

Sample
The sample was prepared by heating a 1:2 molar mixture of $NiCO_3$ and $H_3PO_4$ at about 700°C for 15 hours. It was reground and heated to 1000°C for 15 hours.

Color
Light yellowish green

Structure
Monoclinic, I2/a(15) or Ia(9), Z=8, [Beucher and Grenier, 1968]. These authors gave the cell in the settings C2/c(15) or Cc(9).

NBS lattice constants of this sample:

a = 11.086(3)Å
b = 8.227(2)
c = 9.832(3)
β = 112.74(3)°

Volume
826.9 $Å^3$

Density
(calculated) 3.480 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 1.7

Additional pattern
1. PDF card 19-835 (Sarver, 1966].

References
Beucher, M. and Grenier, J. C. (1968). Mater. Res. Bull. 3, 643.
Sarver, J. F. (1966). Trans. Brit. Ceram. Soc. 65, 191.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.39 | 7 | 110 | 13.84 |
| 6.08 | 50 | 011 | 14.55 |
| 5.11 | 3 | 200 | 17.33 |
| 4.53 | 20 | $\bar{2}11$ | 19.56 |
| 4.321 | 3 | $\bar{2}02$ | 20.54 |
| 4.209 | 40 | $\bar{1}12$ | 21.09 |
| 3.711 | 5 | $\bar{1}21$ | 23.96 |
| 3.493 | 19 | 211 | 25.48 |
| 3.339 | 30 | 112 | 26.68 |
| 3.205 | 11 | 220 | 27.81 |
| 3.148 | 30 | 310 | 28.33 |
| 3.049 | 4 | 022 | 29.27 |
| 2.979 | 100 | $\bar{2}22$ | 29.97 |
| 2.836 | 25 | 013 | 31.52 |
| 2.748 | 2 | $\bar{3}21$ | 32.56 |
| 2.650 | 2 | 130 | 33.80 |
| 2.612 | 4 | $\bar{4}11$ | 34.31 |
| 2.557 | 25 | 400,$\bar{1}23$ | 35.06 |
| 2.451 | 4 | $\bar{2}31$ | 36.64 |
| 2.359 | 25 | $\bar{3}23$ | 38.11 |
| 2.263 | 8 | $\bar{3}14$ | 39.81 |
| 2.220 | 2 | 123 | 40.60 |
| 2.165 | 13 | 411 | 41.69 |
| 2.135 | 3 | 330,$\bar{5}12$ | 42.29 |
| 2.106 | 3 | $\bar{2}24$ | 42.90 |
| 2.081 | 20 | $\bar{2}33$ | 43.44 |
| 2.057 | 4 | 040 | 43.99 |
| 2.001 | 2 | $\bar{1}41$ | 45.28 |
| 1.936 | 4 | 141 | 46.90 |
| 1.929 | 7 | 402,$\bar{5}21$ | 47.07 |
| 1.912 | 5 | $\bar{2}15$ | 47.52 |
| 1.882 | 2 | $\bar{5}23$ | 48.33 |
| 1.856 | 2 | $\bar{2}42$ | 49.03 |
| 1.848 | 2 | $\bar{6}02$ | 49.26 |
| 1.8102 | 3 | $\bar{4}15$ | 50.37 |
| 1.7968 | 3 | $\bar{3}41$ | 50.77 |
| 1.7857 | 4 | $\bar{3}34$ | 51.11 |
| 1.7638 | 2 | $\bar{6}11$ | 51.79 |
| 1.7392 | 9 | $\bar{1}43$,233 + | 52.58 |
| 1.7215 | 5 | $\bar{5}32$ | 53.16 |
| 1.6858 | 7 | $\bar{6}22$,521 | 54.38 |
| 1.6740 | 3 | $\bar{3}43$,242 | 54.79 |
| 1.6704 | 3 | 224 | 54.92 |
| 1.6193 | 7 | 051 | 56.81 |
| 1.5976 | 10 | $\bar{2}35$ | 57.65 |
| 1.5759 | 1 | $\bar{2}44$,$\bar{2}51$ | 58.52 |
| 1.5577 | 2 | $\bar{1}16$ | 59.27 |
| 1.5534 | 4 | 125 | 59.45 |
| 1.5233 | 7 | 044 | 60.74 |

# Potassium barium chromium oxide, $K_2Ba(CrO_4)_2$

Sample
The sample was prepared by heating $K_2Cr_2O_7$ and $BaCO_3$ in a 1:1 molar ratio at 750 °C for 1 hour followed by grinding and heating for 18 hours at 750 °C.

Color
Light greenish yellow

Structure
Hexagonal, $R\bar{3}m(166)$. Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double sulfates and chromates [Schwarz, 1966]. The structure of $Sr_3(PO_4)_2$ was determined by Wilhelmi [1967] and $(NH_4)_2Pb(SO_4)_2$ was determined by Møller [1954].

NBS lattice constants of this sample:

a = 5.7292(5) Å
c = 21.512(3)

Volume
611.51 $Å^3$

Density
(calculated) 3.645 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 3.3(2)

Additional pattern
1. PDF card 19-937 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.
Wilhelmi, K.-A., (1967). Ark. Kemi 26, 157.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.16 | 15 | 003 | 12.36 |
| 4.83 | 4 | 101 | 18.36 |
| 4.503 | 30 | 012 | 19.70 |
| 3.642 | 3 | 104 | 24.42 |
| 3.590 | 2 | 006 | 24.78 |
| 3.251 | 100 | 015 | 27.41 |
| 2.864 | 70 | 110 | 31.21 |
| 2.661 | 14 | 113 | 33.65 |
| 2.612 | 8 | 107 | 34.31 |
| 2.464 | 2 | 021 | 36.43 |
| 2.416 | 3 | 202 | 37.18 |
| 2.390 | 7 | 009 | 37.61 |
| 2.252 | 11 | 024 | 40.00 |
| 2.238 | 8 | 116 | 40.26 |
| 2.149 | 30 | 205 | 42.01 |
| 1.973 | 20 | 1·0·10 | 45.95 |
| 1.868 | 2 | 211 | 48.70 |
| 1.848 | 4 | 122 | 49.27 |
| 1.836 | 5 | 119 | 49.60 |
| 1.8234 | 3 | 208 | 49.98 |
| 1.7926 | 3 | 0·0·12 | 50.90 |
| 1.7188 | 15 | 125 | 53.25 |
| 1.6538 | 9 | 300 | 55.52 |
| 1.6253 | 7 | 0·2·10 | 56.58 |
| 1.6118 | 3 | 303 | 57.10 |
| 1.6007 | 2 | 217 | 57.53 |
| 1.5200 | 3 | 1·1·12 | 60.90 |
| 1.5017 | 2 | 306 | 61.72 |
| 1.4676 | 2 | 0·1·14 | 63.32 |
| 1.4321 | 9 | 220 | 65.08 |
| 1.4134 | 10 | 2·1·10 | 66.05 |
| 1.4045 | 1 | 223 | 66.52 |
| 1.3766 | 2 | 0·2·13 | 68.05 |
| 1.3731 | 1 | 131 | 68.25 |
| 1.3650 | 2 | 312 | 68.71 |
| 1.3600 | 2 | 309 | 69.00 |
| 1.3533 | 1 | 1·2·11 | 69.39 |
| 1.3108 | 5 | 315 | 71.98 |
| 1.2823 | 7 | 1·1·15 | 73.84 |
| 1.2561 | 1 | 137 | 75.65 |
| 1.2289 | 2 | 229 | 77.63 |
| 1.2260 | 1 | 0·1·17 | 77.85 |
| 1.2157 | 2 | 3·0·12 | 78.64 |

# Potassium barium molybdenum oxide, $K_2Ba(MoO_4)_2$

Sample
The sample was made by melting together $MoO_3$, $K_2CO_3$ and $BaCO_3$ in a molar ratio of 2:1:1, followed by grinding and reheating.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $K_2Pb(SO_4)_2$, $Sr_3(PO_4)_2$ and other double chromates and sulfates [Trunin et al., 1975]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$a = 6.0051(4)$ Å
$c = 21.324(2)$

Volume
665.96 Å$^3$

Density
(calculated) 4.004 g/cm$^3$

Reference intensity
$I/I_{corundum} = 4.2(3)$

Additional pattern
1. Trunin et al. [1975].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Trunin, A. S., Shter, G. E., and Serezhkin, V. N., (1975). Russ. J. Inorg. Chem. 20, 1227.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.104 | 9 | 003 | 12.45 |
| 5.055 | 7 | 101 | 17.53 |
| 4.677 | 20 | 012 | 18.96 |
| 3.719 | 4 | 104 | 23.91 |
| 3.552 | 3 | 006 | 25.05 |
| 3.296 | 100 | 015 | 27.03 |
| 3.001 | 90 | 110 | 29.75 |
| 2.765 | 8 | 113 | 32.35 |
| 2.629 | 7 | 107 | 34.08 |
| 2.370 | 1 | 009 | 37.94 |
| 2.338 | 2 | 024 | 38.48 |
| 2.220 | 35 | 205 | 40.61 |
| 1.973 | 25 | 1·0·10 | 45.97 |
| 1.933 | 2 | 122 | 46.96 |
| 1.861 | 2 | 208,119 | 48.90 |
| 1.844 | 2 | 214 | 49.37 |
| 1.785 | 20 | 125 | 51.12 |
| 1.734 | 11 | 300 | 52.76 |
| 1.684 | 2 | 303 | 54.43 |
| 1.649 | 9 | 0·2·10 | 55.70 |
| 1.530 | 3 | 1·1·12 | 60.46 |
| 1.5009 | 8 | 220 | 61.76 |
| 1.4450 | 10 | 2·1·10 | 64.43 |
| 1.4295 | 2 | 312 | 65.21 |
| 1.4214 | 2 | 0·0·15 | 65.63 |
| 1.3664 | 6 | 315 | 68.63 |
| 1.3036 | 2 | 137 | 72.44 |
| 1.2852 | 7 | 1·1·15 | 73.65 |
| 1.2438 | 4 | 045 | 76.53 |
| 1.1945 | 4 | 1·3·10 | 80.31 |
| 1.1860 | 2 | 0·2·16,232 | 81.01 |
| 1.1491 | 4 | 235 | 84.19 |
| 1.1351 | 4 | 410 | 85.47 |
| 1.1206 | 2 | 413 | 86.85 |
| 1.1106 | 3 | 327 | 87.83 |
| 1.0993 | 4 | 3·0·15 | 88.97 |
| 1.0445 | 2 | 0·1·20 | 95.04 |
| 1.0323 | 2 | 2·2·15 | 96.52 |

# Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$

Sample
The sample was prepared by mixing equal volumes of saturated aqueous solutions of $CaSO_4$ and $K_2SO_4$, and evaporating slowly at room temperature. The first crystals formed were used. The crystals were acicular.

Color
Colorless

Optical data
$N_\alpha$=1.500, $N_\gamma$=1.518 [Aruja, 1958].

Structure
Monoclinic, $P2_1/m$ (11), Z=2 [Laszkiewicz, 1936] The structure of $K_2Ca(SO_4)_2 \cdot H_2O$ has been refined by Corazza and Sabelli[1967] and by Gorogotskaya et al. [1968].

NBS lattice constants of this sample

a = 9.777(2)Å
b = 7.147(2)
c = 6.250(2)
β = 104.01(2)°

Volume
423.7Å$^3$

Density
(calculated) 2.574 g/cm$^3$

Reference intensity
$I/I_{corundum}$ = 1.05(6)

Additional patterns
1. PDF card 11-117 [Aruja, 1958],

2. Baynham and Raistrick [1960].

References

Aruja, E. (1958). Mineral Mag. 31, 943.
Baynham, J. W. and Raistrick, B. (1960). In Chemistry and Technology of Fertilizers (Reinhold, N. Y.). ACS Monogr. Ser. 148, Chap. 21, p. 358.
Corazza, E. and Sabelli, K. (1967). Z. Krist. 124, 398.
Gorogotskaya, L. I., Podberezskaya, N. V. and Borisov, S. V. (1968). Zh. Strukt. Khim., SSSR, 9 #1, 86.
Laszkiewicz, A. (1936). Arch. Mineral. 12, 8.


CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 9.49 | 40 | 100 | 9.31 |
| 5.71 | 55 | 110 | 15.51 |
| 4.74 | 16 | 200 | 18.71 |
| 4.624 | 40 | 011 | 19.18 |
| 4.496 | 30 | $\bar{1}11$ | 19.73 |
| 3.954 | 20 | 210 | 22.47 |
| 3.887 | 30 | 111 | 22.86 |
| 3.572 | 30 | 020 | 24.91 |
| 3.347 | 35 | 120 | 26.61 |
| 3.165 | 75 | 300 | 28.17 |
| 3.114 | 17 | $\bar{3}01,\bar{1}02$ | 28.64 |
| 3.036 | 35 | 002 | 29.40 |
| 2.891 | 30 | $\bar{2}02,310$ | 30.91 |
| 2.855 | 100 | $\bar{1}12,220$ | 31.31 |
| 2.827 | 50 | 121 | 31.62 |
| 2.791 | 20 | 012 | 32.04 |
| 2.741 | 55 | $\bar{2}21$ | 32.64 |
| 2.704 | 15 | 102 | 33.10 |
| 2.560 | 2 | 301 | 35.02 |
| 2.513 | 30 | $\bar{3}02$ | 35.70 |
| 2.447 | 7 | 221 | 36.69 |
| 2.411 | 8 | 311 | 37.26 |
| 2.371 | 20 | 400,$\bar{3}12$ | 37.91 |
| 2.355 | 25 | $\bar{3}21$ | 38.18 |
| 2.312 | 16 | 022,130 | 38.93 |
| 2.288 | 7 | $\bar{4}11$ | 39.34 |
| 2.250 | 4 | 410,$\bar{2}22$ | 40.04 |
| 2.129 | 5 | 230 | 42.42 |
| 2.081 | 14 | 321,$\bar{2}31$ | 43.46 |
| 2.046 | 17 | $\bar{2}03,\bar{4}12$ | 44.23 |
| 2.002 | 9 | $\bar{4}21$ | 45.27 |
| 1.974 | 8 | 420 | 45.90 |
| 1.965 | 25 | 302 | 46.15 |
| 1.9498 | 20 | $\bar{5}01$ | 46.54 |
| 1.9447 | 20 | 013,231 | 46.67 |
| 1.9028 | 12 | 330 | 47.76 |
| 1.8968 | 13 | 500,$\bar{3}31$ | 47.92 |
| 1.8924 | 12 | $\bar{1}32$ | 48.04 |
| 1.8333 | 6 | 510,$\bar{4}22$ | 49.69 |
| 1.7870 | 20 | 132,040 | 51.07 |
| 1.7763 | 7 | 421,$\bar{2}23$ | 51.40 |
| 1.7444 | 4 | 331 | 52.41 |
| 1.6755 | 7 | 520 | 54.74 |
| 1.6293 | 2 | $\bar{6}01$ | 56.43 |
| 1.5812 | 6 | $\bar{4}23,600$ | 58.31 |
| 1.5559 | 11 | 340 | 59.35 |
| 1.5436 | 5 | 610 | 59.87 |
| 1.5293 | 7 | $\bar{6}12$ | 60.49 |
| 1.4781 | 4 | 133 | 62.82 |
| 1.4518 | 8 | $\bar{5}23$ | 64.09 |

Potassium calcium sulfate hydrate (syngenite), $K_2Ca(SO_4)_2 \cdot H_2O$ - (continued)

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.4466 | 6 | $60\bar{1},\bar{4}04$ | 64.35 |
| 1.4278 | 5 | $\bar{2}24,\bar{1}24$ + | 65.30 |
| 1.3964 | 3 | $\bar{7}0\bar{1},\bar{6}13$ | 66.96 |
| 1.3701 | 4 | $\bar{4}42$ | 68.42 |
| 1.3494 | 6 | 522 | 69.62 |
| 1.3413 | 4 | $62\bar{1}$ | 70.10 |
| 1.3314 | 4 | $710,\bar{5}14$ | 70.70 |
| 1.3217 | 8 | $342,\bar{5}33$ | 71.30 |
| 1.3085 | 5 | $\bar{3}43$ | 72.13 |
| 1.2803 | 5 | $\bar{3}34$ | 73.98 |
| 1.2669 | 3 | $\bar{5}24$ | 74.89 |

# Potassium iron chloride hydrate (erythrosiderite), $K_2FeCl_5 \cdot H_2O$

Sample
The sample was made by slow evaporation at room temperature of an acid solution of KCl and $FeCl_3$.

Optical Data
Biaxial (+), $N_\alpha = 1.712$, $N_\beta = 1.75$, $N_\gamma = 1.795$
2V is medium large.

Color
Deep reddish orange

Structure
Orthorhombic, Pmnb (62), Z=4, isostructural with $(NH_4)_2FeCl_5 \cdot H_2O$. The structure was determined by Bellanca [1947].

NBS lattice constants of this sample:

a = 9.706(3)Å
b = 13.585(3)
c = 7.018(1)

Volume
925.3 Å

Density
(calculated) 2.364 g/cm$^3$

Reference intensity
$I/I_{corundum} = 1.9$

Additional patterns
1. PDF card 25-1160, natural mineral [Mandarino, Toronto, Ontario].

Reference
Bellanca, A. (1947). Ric. Sci. Ricostr. 17, 1360.

CuK$\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 5.68 | 35 | 101 | 15.59 |
| 5.566 | 40 | 120 | 15.91 |
| 5.248 | 4 | 111 | 16.88 |
| 4.878 | 14 | 021 | 18.17 |
| 3.832 | 2 | 211 | 23.19 |
| 3.541 | 2 | 131 | 25.13 |
| 3.507 | 2 | 002 | 25.38 |
| 3.440 | 10 | 221 | 25.88 |
| 3.397 | 12 | 012,040 | 26.21 |
| 3.208 | 2 | 112,140 | 27.79 |
| 3.056 | 14 | 041 | 29.20 |
| 2.993 | 19 | 231 | 29.83 |
| 2.969 | 5 | 122 | 30.07 |
| 2.934 | 8 | 301 | 30.44 |
| 2.920 | 10 | 320 | 30.59 |
| 2.841 | 16 | 202 | 31.46 |
| 2.782 | 100 | 212,240 | 32.15 |
| 2.589 | 3 | 241 | 34.62 |
| 2.440 | 25 | 042 | 36.81 |
| 2.427 | 40 | 400 | 37.01 |
| 2.365 | 2 | 142 | 38.02 |
| 2.306 | 2 | 013 | 39.02 |
| 2.244 | 3 | 322,113 | 40.16 |
| 2.211 | 4 | 023 | 40.77 |
| 2.180 | 5 | 242 | 41.39 |
| 2.149 | 12 | 052 | 42.00 |
| 2.099 | 6 | 152 | 43.07 |
| 2.078 | 4 | 033 | 43.51 |
| 2.032 | 8 | 133 | 44.55 |
| 1.995 | 2 | 351 | 45.43 |
| 1.970 | 6 | 261 | 46.04 |
| 1.911 | 3 | 233 | 47.54 |
| 1.902 | 6 | 062,441 | 47.79 |
| 1.890 | 3 | 143 | 48.10 |
| 1.872 | 8 | 501,071 | 48.61 |
| 1.868 | 6 | 162,520 | 48.72 |
| 1.826 | 12 | 432,323 | 49.91 |
| 1.789 | 4 | 352 | 51.01 |
| 1.7711 | 3 | 262 | 51.56 |
| 1.7484 | 3 | 333 | 52.28 |
| 1.7404 | 5 | 014 | 52.54 |
| 1.7209 | 10 | 442 | 53.18 |
| 1.7123 | 4 | 114 | 53.47 |
| 1.6982 | 6 | 072,080 | 53.95 |
| 1.6730 | 4 | 172,180 + | 54.83 |
| 1.6560 | 2 | 460,343 | 55.44 |
| 1.6500 | 4 | 081,204 | 55.66 |
| 1.6392 | 3 | 541 | 56.06 |
| 1.6349 | 5 | 034,423 | 56.22 |
| 1.6084 | 8 | 452 | 57.23 |
| 1.5621 | 3 | 281 | 59.09 |

# Potassium lead chromium oxide, $K_2Pb(CrO_4)_2$

Sample
The sample was prepared by melting a 1:1 molar mixture of $K_2CrO_4$ and $PbCrO_4$.

Color
Strong yellow

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3PO_4$ and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was determined by Møller [1954].

NBS lattice constants of this sample:

a = 5.7173(7) Å
c = 21.031(3)

Volume
595.35 $Å^3$

Density
(calculated) 4.329 $g/cm^3$

Reference intensity
$I/I_{corundum} = 3.8(2)$

Additional pattern
1. PDF card 19-971 [Schwarz, 1966]

References
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 345, 230.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.99 | 30 | 003 | 12.65 |
| 4.82 | 19 | 101 | 18.39 |
| 4.47 | 40 | 012 | 19.83 |
| 3.604 | 8 | 104 | 24.68 |
| 3.505 | 2 | 006 | 25.39 |
| 3.204 | 100 | 015 | 27.82 |
| 2.859 | 85 | 110 | 31.26 |
| 2.647 | 20 | 113 | 33.84 |
| 2.571 | 8 | 107 | 34.87 |
| 2.457 | 4 | 021 | 36.54 |
| 2.336 | 6 | 009 | 38.50 |
| 2.240 | 11 | 024 | 40.23 |
| 2.216 | 11 | 116 | 40.69 |
| 2.133 | 30 | 205 | 42.34 |
| 1.935 | 19 | 1·0·10 | 46.92 |
| 1.863 | 4 | 211 | 48.83 |
| 1.842 | 5 | 122 | 49.45 |
| 1.809 | 5 | 119 | 50.41 |
| 1.802 | 5 | 208 | 50.62 |
| 1.764 | 2 | 214 | 51.80 |
| 1.753 | 2 | 0·0·12 | 52.13 |
| 1.7102 | 19 | 125 | 53.54 |
| 1.6508 | 9 | 300 | 55.63 |
| 1.6066 | 7 | 303 | 57.30 |
| 1.6033 | 7 | 0·2·10 | 57.43 |
| 1.5884 | 3 | 217 | 58.02 |
| 1.4935 | 3 | 1·1·12,306 | 62.10 |
| 1.4380 | 2 | 0·1·14 | 64.78 |
| 1.4293 | 7 | 220 | 65.22 |
| 1.3978 | 10 | 2·1·10 | 66.88 |
| 1.3621 | 2 | 312 | 68.88 |
| 1.3053 | 6 | 315 | 72.33 |
| 1.2586 | 6 | 1·1·15 | 75.47 |

# Potassium lead molybdenum oxide, $K_2Pb(MoO_4)_2$

Sample
The sample was prepared by melting together $K_2CO_3$, $PbCO_3$ and $MoO_3$, at about 850 °C.

Color
Yellowish white

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3. The similarity of the cell size, powder patterns, and chemistry of $K_2Pb(MoO_4)_2$, $Sr_3(PO_4)_2$, $K_2Pb(SO_4)_2$ (palmierite), and $(NH_4)_2Pb(SO_4)_2$ strongly suggests an isostructural relationship. The structure of $(NH_4)_2Pb(SO_4)_2$ has been studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.9853(2) Å
c = 20.987(1)

Polymorphism
Belyaev [1961] reports a polymorphic transformation of $K_2Pb(MoO_4)_2$ at 765 °C. No evidence of this was seen in the present work.

Volume
651.09 $Å^3$

Density
(calculated) 4.631 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 4.0(3)

References
Belyaev, I.N. (1961). Russ. J. Inorg. Chem. 6, 602.
Møller, C. K. (1954). Acta Chem. Scand. 8, 81.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.99 | 25 | 003 | 12.66 |
| 4.648 | 40 | 012 | 19.08 |
| 3.687 | 2 | 104 | 24.12 |
| 3.262 | 100 | 015 | 27.32 |
| 2.993 | 85 | 110 | 29.83 |
| 2.752 | 18 | 113 | 32.51 |
| 2.595 | 8 | 107 | 34.54 |
| 2.332 | 3 | 009 | 38.57 |
| 2.325 | 3 | 024 | 38.70 |
| 2.274 | 3 | 116 | 39.60 |
| 2.205 | 30 | 205 | 40.89 |
| 1.960 | 4 | 027 | 46.28 |
| 1.945 | 18 | 1·0·10 | 46.65 |
| 1.925 | 7 | 122 | 47.17 |
| 1.843 | 3 | 208 | 49.41 |
| 1.7750 | 25 | 125 | 51.44 |
| 1.7485 | 3 | 0·0·12 | 52.28 |
| 1.7279 | 12 | 300 | 52.95 |
| 1.6775 | 3 | 303 | 54.67 |
| 1.6397 | 4 | 217 | 56.04 |
| 1.6312 | 7 | 0·2·10 | 56.36 |
| 1.5694 | 2 | 128 | 58.79 |
| 1.5099 | 3 | 1·1·12 | 61.35 |
| 1.4961 | 8 | 220 | 61.98 |
| 1.4632 | 2 | 223 | 63.53 |
| 1.4398 | 5 | 0·1·14 | 64.69 |
| 1.4319 | 9 | 2·1·10 | 65.09 |
| 1.4245 | 4 | 312 | 65.47 |
| 1.3991 | 2 | 0·0·15 | 66.81 |
| 1.3602 | 8 | 315 | 68.99 |
| 1.2961 | 2 | 137 | 72.93 |
| 1.2675 | 4 | 1·1·15 | 74.85 |
| 1.2382 | 3 | 045 | 76.94 |
| 1.2292 | 1 | 3·0·12 | 77.61 |
| 1.2010 | 1 | 0·1·17 | 79.79 |
| 1.1860 | 5 | 1·3·10 | 81.01 |
| 1.1619 | 1 | 048 | 83.05 |
| 1.1442 | 5 | 235 | 84.63 |
| 1.1368 | 3 | 2·2·12 | 85.31 |
| 1.1312 | 3 | 410 | 85.84 |
| 1.1166 | 1 | 413 | 87.24 |
| 1.1054 | 2 | 327 | 88.35 |
| 1.1028 | 3 | 4·0·10 | 88.61 |
| 1.0874 | 2 | 3·0·15 | 90.21 |

# Potassium lead sulfate (palmierite), $K_2Pb(SO_4)_2$

Sample
The sample was prepared by melting a 1:1 molar mixture of $K_2SO_4$ and $PbSO_4$, grinding and reheating at 450 °C overnight.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample

a = 5.4950(6) Å
c = 20.849(4)

Volume
545.18 $Å^3$

Density
(calculated) 4.363 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 2.77(10)

Additional pattern
1. PDF card 20-902 [Schwarz, 1966]

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H. (1966). Z. Anorg. Allg. Chem. 344, 41.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.948 | 35 | 003 | 12.73 |
| 4.641 | 25 | 101 | 19.11 |
| 4.333 | 45 | 012 | 20.48 |
| 3.515 | 18 | 104 | 25.32 |
| 3.477 | 3 | 006 | 25.60 |
| 3.138 | 100 | 015 | 28.42 |
| 2.749 | 70 | 110 | 32.54 |
| 2.557 | 35 | 113 | 35.07 |
| 2.526 | 13 | 107 | 35.51 |
| 2.366 | 9 | 021 | 38.00 |
| 2.318 | 10 | 202,009 | 38.82 |
| 2.287 | 3 | 018 | 39.36 |
| 2.166 | 25 | 024 | 41.67 |
| 2.156 | 30 | 116 | 41.86 |
| 2.068 | 35 | 205 | 43.74 |
| 1.910 | 25 | 1·0·10 | 47.57 |
| 1.860 | 2 | 027 | 48.94 |
| 1.792 | 10 | 211 | 50.92 |
| 1.772 | 20 | 122,119 | 51.54 |
| 1.760 | 7 | 0·1·11 | 51.92 |
| 1.7575 | 8 | 208 | 51.99 |
| 1.7373 | 4 | 0·0·12 | 52.64 |
| 1.7002 | 3 | 214 | 53.88 |
| 1.6516 | 20 | 125 | 55.60 |
| 1.5861 | 11 | 300 | 58.11 |
| 1.5684 | 8 | 0·2·10 | 58.83 |
| 1.5464 | 5 | 303 | 59.75 |
| 1.5397 | 4 | 217 | 60.04 |
| 1.5195 | 2 | 1·0·13 | 60.92 |
| 1.4823 | 3 | 2·0·11 | 62.62 |
| 1.4802 | 3 | 128 | 62.72 |
| 1.4686 | 5 | 1·1·12 | 63.27 |
| 1.4428 | 6 | 306 | 64.54 |
| 1.4212 | 3 | 0·1·14 | 65.64 |
| 1.3900 | 2 | 0·0·15 | 67.31 |
| 1.3734 | 10 | 220 | 68.23 |
| 1.3617 | 14 | 2·1·10 | 68.90 |
| 1.3479 | 2 | 223 | 69.71 |
| 1.3296 | 2 | 0·2·13 | 70.81 |
| 1.3169 | 1 | 131 | 71.60 |
| 1.3088 | 3 | 312,309 | 72.11 |
| 1.3046 | 3 | 1·2·11 | 72.38 |
| 1.2792 | 2 | 134 | 74.05 |
| 1.2622 | <1 | 2·0·14 | 75.22 |
| 1.2582 | 9 | 315 | 75.50 |
| 1.2403 | 13 | 1·1·15 | 76.79 |
| 1.2067 | 2 | 137 | 79.34 |
| 1.1974 | 2 | 2·1·13 | 80.08 |
| 1.1878 | 2 | 401,0·1·17 | 80.86 |
| 1.1820 | 3 | 042 | 81.34 |

# Potassium strontium sulfate (kalistrontite), $K_2Sr(SO_4)_2$

Sample
Two and one-half grams of $SrCl_2 \cdot 6H_2O$ in 10 mL $H_2O$ was added dropwise to 20 g $K_2SO_4$ in 100 mL $H_2O$ at the boiling point and refluxed with stirring for 4 days. The precipitate was filtered at the boiling point, squeezed on blotting paper and dried in dessicator. The crystallinity was improved by heating the precipitate to 600 °C for 3 days.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.4630(3) Å
c = 20.843(1)

Volume
538.73 $Å^3$

Density
(calculated) 3.310 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 3.3(2)

Additional patterns
1. PDF card 15-123 Voronova [1962].
2. PDF card 19-996 Schwarz [1966].


References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.
Voronova, M. L., (1962). Zap. Vses. Mineral. Obshchest. 91, 712.


$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.94 | 15 | 003 | 12.75 |
| 4.617 | 1 | 101 | 19.21 |
| 4.308 | 17 | 012 | 20.60 |
| 3.472 | 1 | 006 | 25.64 |
| 3.128 | 100 | 015 | 28.51 |
| 2.731 | 65 | 110 | 32.77 |
| 2.543 | 11 | 113 | 35.27 |
| 2.520 | 4 | 107 | 35.60 |
| 2.352 | 2 | 021 | 38.24 |
| 2.316 | 8 | 009 | 38.85 |
| 2.308 | 6 | 202 | 39.00 |
| 2.153 | 17 | 024 | 41.92 |
| 2.148 | 19 | 116 | 42.03 |
| 2.0576 | 25 | 205 | 43.97 |
| 1.9077 | 18 | 1·0·10 | 47.63 |
| 1.7818 | 3 | 211 | 51.23 |
| 1.7664 | 5 | 119 | 51.71 |
| 1.7622 | 2 | 122 | 51.84 |
| 1.7516 | 3 | 208 | 52.18 |
| 1.7364 | 3 | 0·0·12 | 52.67 |
| 1.6915 | <1 | 214 | 54.18 |
| 1.6435 | 12 | 125 | 55.90 |
| 1.5772 | 7 | 300 | 58.47 |
| 1.5641 | 5 | 0·2·10 | 59.01 |
| 1.5376 | 2 | 303 | 60.13 |
| 1.4657 | 1 | 1·1·12 | 63.41 |
| 1.4358 | 2 | 306 | 64.89 |
| 1.4201 | 1 | 0·1·14 | 65.70 |
| 1.3892 | 2 | 0·0·15 | 67.35 |
| 1.3655 | 8 | 220 | 68.68 |
| 1.3570 | 9 | 2·1·10 | 69.17 |
| 1.3400 | 1 | 223 | 70.18 |
| 1.3273 | 1 | 0·2·13 | 70.95 |
| 1.3033 | 1 | 309 | 72.46 |
| 1.3007 | 2 | 1·2·11 | 72.63 |
| 1.2723 | <1 | 134 | 74.52 |
| 1.2513 | 5 | 315 | 75.99 |
| 1.2384 | 8 | 1·1·15 | 76.93 |
| 1.2008 | <1 | 137 | 79.81 |
| 1.1765 | 1 | 229 | 81.80 |
| 1.1677 | <1 | 3·0·12 | 82.55 |
| 1.1533 | <1 | 404 | 83.81 |
| 1.1441 | 1 | 1·2·14 | 84.64 |
| 1.1410 | 1 | 0·2·16 | 84.93 |
| 1.1379 | 2 | 045 | 85.21 |
| 1.1105 | 3 | 1·3·10 | 87.84 |
| 1.0737 | 1 | 2·2·12 | 91.68 |
| 1.0661 | 1 | 1·1·18 | 92.53 |
| 1.0506 | 3 | 235 | 94.31 |
| 1.0426 | 4 | 3·0·15 | 95.26 |
| 1.0324 | 2 | 410 | 96.51 |
| 1.0287 | 1 | 4·0·10 | 96.97 |
| 1.0210 | 1 | 413 | 97.97 |
| 1.0180 | 1 | 0·1·20 | 98.35 |

# Rubidium barium chromium oxide, $Rb_2Ba(CrO_4)_2$

Sample
The sample was prepared by heating a 1:1 molar mixture of $Rb_2Cr_2O_7$ and $BaCO_3$ together at 750° for 1 hour. This was followed by grinding, and reheating at 750° for 48 hours.

Color
Light greenish yellow

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double sulfates, chromates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

$a = 5.8107(6)$ Å
$c = 22.210(3)$

Volume
649.4 $Å^3$

Density
(calculated) 4.144 $g/cm^3$

Reference Intensity
$I/I_{corundum} = 5.8(2)$

Additional pattern
1. PDF card 19-1066 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.

$CuK\alpha_1$ $\lambda$ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.39 | 2 | 003 | 11.96 |
| 4.90 | 6 | 101 | 18.09 |
| 4.58 | 4 | 012 | 19.38 |
| 3.731 | 4 | 104 | 23.83 |
| 3.326 | 100 | 015 | 26.78 |
| 2.905 | 65 | 110 | 30.75 |
| 2.705 | 2 | 113 | 33.09 |
| 2.683 | 2 | 107 | 33.37 |
| 2.500 | 2 | 021 | 35.89 |
| 2.467 | 5 | 009 | 36.39 |
| 2.455 | 4 | 202 | 36.58 |
| 2.430 | 2 | 018 | 36.97 |
| 2.291 | 9 | 024 | 39.29 |
| 2.287 | 12 | 116 | 39.37 |
| 2.189 | 25 | 205 | 41.21 |
| 2.031 | 20 | 1·0·10 | 44.57 |
| 1.972 | 1 | 027 | 45.99 |
| 1.895 | 2 | 211 | 47.96 |
| 1.881 | 5 | 119 | 48.34 |
| 1.876 | 3 | 122 | 48.49 |
| 1.850 | 1 | 0·0·12 | 49.20 |
| 1.799 | 1 | 214 | 50.70 |
| 1.748 | 15 | 125 | 52.28 |
| 1.677 | 7 | 300 | 54.68 |
| 1.665 | 8 | 0·2·10 | 55.10 |
| 1.528 | 1 | 306 | 60.56 |
| 1.513 | 1 | 0·1·14 | 61.19 |
| 1.480 | 2 | 0·0·15 | 62.71 |
| 1.453 | 7 | 220 | 64.02 |
| 1.4448 | 10 | 2·1·10 | 64.44 |
| 1.3869 | 1 | 309 | 67.48 |
| 1.3314 | 5 | 315 | 70.70 |
| 1.3196 | 8 | 1·1·15 | 71.43 |
| 1.2520 | 2 | 229 | 75.94 |
| 1.2102 | 3 | 045 | 79.06 |
| 1.1819 | 4 | 1·3·10 | 81.35 |

# Rubidium iron chloride hydrate, $Rb_2FeCl_5 \cdot H_2O$

Sample
The sample was prepared by slow evaporation at room temperature. Since the material was incongruently soluble, a 1:1 molar aqueous solution of RbCl and $FeCl_3$ was prepared with some additional HCl. The first crystals formed were used.

Color
Deep reddish orange

Structure
Orthorhombic, Pmnb (62), Z = 4, isostructural with $K_2FeCl_5 \cdot H_2O$ and $(NH_4)_2FeCl_5 \cdot H_2O$. The structure of $K_2FeCl_5 \cdot H_2O$ was determined by Bellanca [1947].

NBS lattice constants of this sample:

a = 9.923(3) Å
b = 13.836(4)
c = 7.092(2)

Volume
973.8 $Å^3$

Density
(calculated) 2.879 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 1.7(2)

Reference
Bellanca, A.,(1947). Rec. Sci. Recostr. 17, 1360.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 6.92 | 6 | 020 | 12.78 |
| 6.31 | 3 | 011 | 14.02 |
| 5.78 | 30 | 101 | 15.33 |
| 5.68 | 30 | 120 | 15.58 |
| 5.34 | 4 | 111 | 16.60 |
| 4.960 | 8 | 200,021 | 17.87 |
| 3.904 | 8 | 211 | 22.76 |
| 3.870 | 4 | 031 | 22.96 |
| 3.602 | 4 | 131 | 24.70 |
| 3.504 | 50 | 221 | 25.40 |
| 3.462 | 25 | 040 | 25.71 |
| 3.436 | 20 | 012 | 25.91 |
| 3.109 | 17 | 041 | 28.69 |
| 3.050 | 30 | 231 | 29.26 |
| 3.006 | 8 | 122 | 29.70 |
| 2.996 | 7 | 301 | 29.80 |
| 2.885 | 25 | 202 | 30.97 |
| 2.836 | 90 | 240 | 31.52 |
| 2.826 | 100 | 212 | 31.63 |
| 2.814 | 70 | 032 | 31.77 |
| 2.635 | 8 | 241 | 33.99 |
| 2.479 | 55 | 400,042 | 36.21 |
| 2.403 | 3 | 142 | 37.40 |
| 2.308 | 2 | 411,060 | 38.99 |
| 2.238 | 3 | 023 | 40.26 |
| 2.218 | 2 | 421 | 40.65 |
| 2.180 | 18 | 052 | 41.38 |
| 2.130 | 6 | 152 | 42.40 |
| 2.108 | 7 | 213 | 42.87 |
| 2.089 | 2 | 431 | 43.28 |
| 2.058 | 5 | 133 | 43.96 |
| 2.010 | 14 | 412 | 45.06 |
| 2.004 | 15 | 261 | 45.20 |
| 1.997 | 9 | 252 | 45.38 |
| 1.940 | 12 | 441 | 46.79 |
| 1.936 | 14 | 233 | 46.88 |
| 1.912 | 7 | 501 | 47.51 |
| 1.860 | 15 | 432 | 48.92 |
| 1.820 | 3 | 352 | 50.07 |
| 1.800 | 2 | 262 | 50.66 |
| 1.776 | 4 | 333 | 51.41 |
| 1.773 | 5 | 004 | 51.50 |
| 1.758 | 8 | 014 | 51.97 |
| 1.753 | 13 | 442 | 52.13 |
| 1.730 | 6 | 080 | 52.88 |
| 1.698 | 3 | 413 | 53.96 |
| 1.679 | 6 | 081,522 | 54.61 |
| 1.6696 | 4 | 204,362 | 54.95 |
| 1.6552 | 5 | 034 | 55.47 |
| 1.6378 | 12 | 452 | 56.11 |

# Rubidium lead chromium oxide, $Rb_2Pb(CrO_4)_2$

Sample
The sample was prepared by melting a mixture of $Rb_2CrO_4$ and $PbCrO_4$, at about 730 °C.

Color
Slight orange yellow

Structure
Hexagonal, $R\bar{3}m(166)$, Z = 3, isostructural with $Sr_3(PO_4)_2$ and many double chromates, sulfates, and selenates [Schwarz, 1966]. The structure of $(NH_4)_2Pb(SO_4)_2$ was studied by Møller [1954].

NBS lattice constants of this sample:

a = 5.8037(4) Å
c = 21.827(3)

Volume
636.70 $Å^3$

Density
(calculated) 4.773 $g/cm^3$

Reference intensity
$I/I_{corundum}$ = 5.3(3)

Additional pattern
1. PDF card 19-1077 [Schwarz, 1966].

References
Møller, C. K., (1954). Acta Chem. Scand. 8, 81.
Schwarz, H., (1966). Z. Anorg. Allg. Chem. 344, 41.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 7.273 | 12 | 003 | 12.16 |
| 4.897 | 25 | 101 | 18.10 |
| 4.567 | 10 | 012 | 19.42 |
| 3.699 | 9 | 104 | 24.04 |
| 3.638 | 4 | 006 | 24.45 |
| 3.296 | 100 | 015 | 27.03 |
| 2.904 | 75 | 110 | 30.76 |
| 2.696 | 7 | 113 | 33.21 |
| 2.650 | 2 | 107 | 33.80 |
| 2.497 | 5 | 021 | 35.93 |
| 2.426 | 5 | 009 | 37.03 |
| 2.283 | 13 | 024 | 39.43 |
| 2.270 | 12 | 116 | 39.68 |
| 2.178 | 25 | 205 | 41.43 |
| 2.002 | 17 | 1·0·10 | 45.26 |
| 1.957 | 2 | 027 | 46.34 |
| 1.892 | 5 | 211 | 48.04 |
| 1.871 | 3 | 122 | 48.63 |
| 1.861 | 5 | 119 | 48.89 |
| 1.849 | 1 | 208 | 49.24 |
| 1.819 | 1 | 0·0·12 | 50.12 |
| 1.794 | 2 | 214 | 50.85 |
| 1.742 | 18 | 125 | 52.49 |
| 1.675 | 8 | 300 | 54.75 |
| 1.648 | 5 | 0·2·10 | 55.73 |
| 1.632 | 1 | 303 | 56.32 |
| 1.558 | 2 | 2·0·11 | 59.26 |
| 1.5216 | 2 | 306 | 60.83 |
| 1.4889 | 2 | 0·1·14 | 62.31 |
| 1.4546 | 7 | 0·0·15 | 63.95 |
| 1.4506 | 6 | 220 | 64.15 |
| 1.4329 | 8 | 2·1·10 | 65.04 |
| 1.3912 | 2 | 131 | 67.24 |
| 1.3784 | 2 | 309 | 67.95 |
| 1.3720 | 2 | 1·2·11 | 68.31 |
| 1.3507 | 1 | 134 | 69.54 |
| 1.3276 | 5 | 315 | 70.93 |
| 1.3008 | 5 | 1·1·15 | 72.62 |
| 1.2447 | 1 | 229 | 76.46 |
| 1.2242 | 1 | 404 | 77.99 |
| 1.2074 | 3 | 045 | 79.28 |
| 1.1747 | 3 | 1·3·10 | 81.95 |
| 1.1519 | <1 | 321 | 83.94 |
| 1.1149 | 2 | 235 | 87.41 |
| 1.0987 | 3 | 3·0·15 | 89.03 |
| 1.0969 | 3 | 410 | 89.22 |

# Sodium magnesium sulfate hydrate (loeweite), $Na_{12}Mg_7(SO_4)_{13}\cdot 15H_2O$

Sample

The sample was prepared by evaporation of an aqueous solution of a 6:7 molar ratio of $Na_2SO_4$ and $MgSO_4$ at 95 °C. The precipitate was filtered off while the solution was hot. The composition of this phase was originally given as $Na_2Mg(SO_4)_2\cdot 2.5H_2O$. It was corrected by Kühn and Ritter [1958]. The sample contained about 15% of bloedite [$Na_2Mg(SO_4)_2\cdot 4H_2O$]. This pattern has been confirmed by computer calculation using structure data from Fang and Robinson [1970]. The sample was colorless.

Intensities

The intensities given in the table have been calculated from the data of Fang and Robinson [1970], and thus represent the intensities which would be obtained from a sample free from bloedite.

Structure

Hexagonal, $R\bar{3}$ (148), Z = 3, isostructural with $Na_{12}Mn_7(SO_4)_{13}\cdot 15H_2O$ [Schneider and Zemann, 1959]. The structure of loeweite was determined by Fang and Robinson [1970].

NBS lattice constants of this sample:

a = 18.866(2) Å
c = 13.434(2)

A least squares refinement based on 43 unique reflections free from bloedite gave lattice constants which did not differ from those above by more than 0.005 A.

Volume

4140.9 $Å^3$

Density

(calculated) 2.364 $g/cm^3$

Reference intensity

$I/I_{corundum} = 0.56(3)$

Additional patterns

1. PDF card 21-1139 [Madsen, 1966]
2. PDF card 24-1107 [Heide, Min. Inst. Jena, 1967]. This pattern has the formula incorrectly given as $Na_2Mg(SO_4)_2\cdot 2.5H_2O$.


References

Fang, J. H., and Robinson, P. D., (1970). Am. Mineralogist 55, 378.

Kuhn, R., and Ritter, K.-H. (1958). Kali Steinsalz 2, 238.

Madsen, B. M., (1966). U. S. Geol. Surv. Prof. Pap. 550B, 125.

Schneider, W. (1960). Z. Anorg. Allg. Chem. 303, 113.

Schneider, W., and Zemann, J. (1959). Beitr. Mineral. Petrogr. 6, 201.


$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 10.37 | 100 | 101 | 8.52 |
| 9.42 | 18 | 110 | 9.38 |
| 6.98 | 26 | 021 | 12.68 |
| 6.21 | 14 | 012 | 14.26 |
| 5.61 | 28 | 211 | 15.78 |
| 5.45 | 32 | 300 | 16.26 |
| 5.19 | 5 | 202 | 17.07 |
| 4.55 | 8 | 122 | 19.49 |
| 4.471 | 10 | 003 | 19.84 |
| 4.294 | 65 | 131 | 20.67 |
| 4.046 | 62 | 113 | 21.95 |
| 3.904 | 2 | 401 | 22.76 |
| 3.759 | 31 | 312 | 23.65 |
| 3.612 | 9 | 321 | 24.63 |
| 3.563 | 4 | 410 | 24.97 |
| 3.493 | 2 | 042 | 25.48 |
| 3.458 | 52 | 303 | 25.74 |
| 3.277 | 45 | 232 | 27.19 |
| 3.251 | 23 | 223 | 27.41 |
| 3.175 | 41 | 051 | 28.08 |
| 3.144 | 10 | 330 | 28.36 |
| 3.109 | 4 | 024 | 28.69 |
| 3.012 | 6 | 241 | 29.64 |
| 2.949 | 3 | 214 | 30.28 |
| 2.942 | 21 | 502 | 30.36 |
| 2.868 | 22 | 511 | 31.16 |
| 2.806 | 17 | 422 | 31.87 |
| 2.790 | 23 | 413 | 32.06 |
| 2.723 | 22 | 600 | 32.86 |
| 2.698 | 47 | 134 | 33.18 |
| 2.635 | 15 | 431 | 34.00 |
| 2.617 | 17 | 520 | 34.24 |
| 2.552 | 1 | 205 | 35.14 |
| 2.499 | 1 | 324 | 35.90 |
| 2.494 | 3 | 342 | 35.98 |
| 2.451 | 10 | 161 | 36.64 |
| 2.356 | 5 | 440 | 38.16 |
| 2.343 | 1 | 054 | 38.39 |
| 2.335 | 5 | 612 | 38.52 |
| 2.311 | 4 | 315 | 38.94 |
| 2.273 | 1 | 244 | 39.62 |
| 2.259 | 2 | 523 | 39.87 |
| 2.211 | 15 | 514 | 40.78 |
| 2.206 | 15 | 072 | 40.87 |
| 2.180 | 6 | 116 | 41.39 |
| 2.163 | 3 | 710 | 41.72 |
| 2.097 | 2 | 434 | 43.10 |
| 2.070 | 9 | 306 | 43.69 |
| 2.066 | 11 | 541 | 43.78 |
| 2.023 | 16 | 226 | 44.76 |

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 1.999 | 8 | 452 | 45.34 |
| 1.954 | 4 | 802 | 46.43 |
| 1.917 | 8 | 354 | 47.38 |
| 1.900 | 4 | 345 | 47.84 |
| 1.896 | 4 | 416 | 47.95 |
| 1.870 | 3 | 633 | 48.65 |
| 1.856 | 1 | 461 | 49.03 |
| 1.839 | 6 | 182 | 49.54 |
| 1.833 | 4 | 217 | 49.69 |
| 1.805 | 4 | 642 | 50.51 |
| 1.783 | 3 | 820 | 51.18 |
| 1.776 | 6 | 544 | 51.42 |
| 1.761 | 3 | 075 | 51.87 |
| 1.739 | 8 | 553,407 | 52.60 |
| 1.716 | 2 | 274 | 53.34 |
| 1.708 | 3 | 327 | 53.61 |
| 1.699 | 5 | 191 | 53.92 |
| 1.694 | 4 | 740 | 54.08 |
| 1.6821 | 3 | 903 | 54.51 |
| 1.6702 | 2 | 018 | 54.93 |
| 1.6557 | 8 | 823,057 | 55.45 |
| 1.6503 | 8 | 455 | 55.65 |
| 1.6448 | 6 | 208 | 55.85 |
| 1.6362 | 5 | 464 | 56.17 |
| 1.6301 | 6 | 247 | 56.40 |
| 1.6100 | 5 | 832 | 57.17 |
| 1.5869 | 4 | 0·10·2 | 58.08 |
| 1.5750 | 5 | 318 | 58.56 |
| 1.5576 | 2 | 185 | 59.28 |

# Sodium manganese sulfate hydrate, $Na_{12}Mn_7(SO_4)_{13}\cdot 15H_2O$

Sample
The sample was prepared by evaporation of an aqueous solution of 4:3 molar mixture of $Na_2SO_4$ and $MnSO_4$ at 95 °C. The crystals were filtered off while the solution was hot.

Color
Pale pink

Optical data
Uniaxial (—), $N_e = 1.501$, $N_o = 1.520$

Structure
Hexagonal, $R\bar{3}$ (148), Z = 3, isostructural with $Na_{12}Mg_7(SO_4)_{13}\cdot 15H_2O$ (loeweite). The structure has been studied by Schneider [1960].

NBS lattice constants of this sample:

a = 19.126(2) Å
b = 13.529(3)

Volume
4285.7 $Å^3$

Density
(calculated) 2.533 $g/cm^3$

Reference intensity
$I/I_{corundum} = 0.66(7)$

Reference
Schneider, W. (1960). Z. Anorg. Allg. Chem. 303, 113.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

| d(Å) | I | hkℓ | 2θ(°) |
|---|---|---|---|
| 10.47 | 55 | 101 | 8.44 |
| 9.57 | 25 | 110 | 9.23 |
| 7.07 | 85 | 021 | 12.51 |
| 6.25 | 35 | 012 | 14.15 |
| 5.683 | 30 | 211 | 15.58 |
| 5.525 | 30 | 300 | 16.03 |
| 4.784 | 20 | 220 | 18.53 |
| 4.595 | 25 | 122 | 19.30 |
| 4.510 | 35 | 003 | 19.67 |
| 4.350 | 80 | 131 | 20.40 |
| 4.079 | 70 | 113 | 21.77 |
| 3.803 | 16 | 312 | 23.37 |
| 3.660 | 30 | 321 | 24.30 |
| 3.616 | 14 | 410 | 24.60 |
| 3.531 | 14 | 042 | 25.21 |
| 3.494 | 80 | 303 | 25.47 |
| 3.312 | 90 | 104,232 | 26.90 |
| 3.282 | 18 | 223 | 27.15 |
| 3.218 | 70 | 051 | 27.70 |
| 3.189 | 18 | 330 | 27.96 |
| 3.132 | 11 | 024 | 28.48 |
| 3.051 | 7 | 241 | 29.25 |
| 2.977 | 35 | 214,502 | 29.99 |
| 2.907 | 55 | 511 | 30.73 |
| 2.843 | 40 | 422 | 31.44 |
| 2.820 | 45 | 413 | 31.70 |
| 2.760 | 50 | 600 | 32.41 |
| 2.723 | 100 | 134,152 | 32.86 |
| 2.669 | 9 | 015,431 | 33.55 |
| 2.651 | 30 | 520 | 33.78 |
| 2.603 | 8 | 333 | 34.43 |
| 2.527 | 10 | 324,342 | 35.50 |
| 2.483 | 9 | 125,161 | 36.14 |
| 2.391 | 9 | 440 | 37.59 |
| 2.367 | 25 | 054,612 | 37.99 |
| 2.329 | 17 | 315,351 | 38.62 |
| 2.285 | 5 | 523 | 39.40 |
| 2.265 | 8 | 045,621 | 39.76 |
| 2.254 | 18 | 006 | 39.96 |
| 2.233 | 55 | 514,072 | 40.36 |
| 2.194 | 11 | 116,710 | 41.11 |
| 2.122 | 6 | 434 | 42.57 |
| 2.113 | 6 | 443 | 42.75 |
| 2.095 | 20 | 505,541 | 43.15 |
| 2.089 | 16 | 306,630 | 43.28 |
| 2.046 | 17 | 425,081 | 44.23 |
| 2.039 | 30 | 226 | 44.39 |
| 2.022 | 15 | 164,452 | 44.78 |
| 2.001 | 6 | 155,271 | 45.29 |
| 1.979 | 8 | 802 | 45.81 |
| 1.973 | 9 | 713 | 45.95 |
| 1.938 | 19 | 354,722 | 46.83 |
| 1.920 | 14 | 107,345 | 47.31 |
| 1.913 | 10 | 416,550 | 47.48 |
| 1.893 | 10 | 633 | 48.01 |
| 1.882 | 4 | 027,461 | 48.33 |
| 1.864 | 6 | 182 | 48.83 |
| 1.846 | 6 | 615,731 | 49.32 |
| 1.841 | 8 | 336,900 | 49.48 |
| 1.829 | 9 | 642 | 49.83 |
| 1.796 | 10 | 544,372 | 50.80 |
| 1.781 | 12 | 137,075 | 51.26 |
| 1.761 | 15 | 553 | 51.89 |
| 1.736 | 4 | 274 | 52.67 |
| 1.722 | 13 | 327,191 | 53.15 |
| 1.717 | 13 | 526,740 | 53.31 |
| 1.704 | 6 | 903 | 53.75 |
| 1.681 | 16 | 814,562 | 54.54 |
| 1.678 | 14 | 823 | 54.66 |
| 1.670 | 12 | 057,455 | 54.94 |
| 1.657 | 12 | 208,464 | 55.40 |
| 1.620 | 8 | 921,725 + | 56.78 |
| 1.608 | 10 | 0·10·2 | 57.24 |
| 1.604 | 7 | 743 | 57.39 |
| 1.586 | 12 | 318,292 | 58.10 |

# Acetanilide, $C_6H_5NHCOCH_3$

Synonym
N - phenylacetamide

Structure
Orthorhombic, Pbca (61), Z = 8. The structure was determined by Brown and Corbridge [1954] and refined by Brown [1966].

Atom positions
All atoms were in general positions.

Lattice constants
a = 19.641 A
b = 9.483
c = 7.979
(published values: a = 19.640, b = 9.483, c = 7.979 [Brown and Corbridge, 1954]).

CD cell: a = 9.483, b = 19.641, c = 7.979, space group Pcab; a/b = 0.4828, c/b = 0.4063

Volume
1486. $A^3$

Density
(measured) 1.206 g/cm$^3$
(calculated) 1.208 g/cm$^3$

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
$C^0$, $H^0$, $N^0$, $O^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.471 \times 10^{-3}$
$I/I_c$ (calculated) = 0.50

Additional pattern
1. PDF card 18-1501 [Billig, B. and Greenberg, B., Polytechnic Inst. of Brooklyn]

References

Brown, C. J. and Corbridge, D. E. C. (1954). Acta Crystallogr. 7, 711.
Brown, C. J. (1966). Acta Crystallogr. 21, 442.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 9.82 | 100 | 2 0 0 | 9.00 |
| 6.82 | 38 | 2 1 0 | 12.98 |
| 5.82 | 81 | 1 1 1 | 15.20 |
| 5.18 | 31 | 2 1 1 | 17.10 |
| 4.91 | 3 | 4 0 0 | 18.06 |
| 4.74 | 6 | 0 2 0 | 18.72 |
| 4.46 | 26 | 3 1 1 | 19.88 |
| 4.36 | 27 | 4 1 0 | 20.36 |
| 4.27 | 5 | 2 2 0 | 20.80 |
| 4.07 | 40 | 0 2 1 | 21.80 |
| 3.99 | 58 | 1 2 1 | 22.26 |
| 3.91 | 29 | 1 0 2 | 22.74 |
| 3.82 | 9 | 4 1 1 | 23.24 |
| 3.76 | 36 | 2 2 1 | 23.62 |
| 3.70 | 73 | 2 0 2 | 24.06 |
| 3.61 | 25 | 1 1 2 | 24.62 |
| 3.44 | 47 | 2 1 2 | 25.86 |
| 3.41 | 8 | 3 0 2 | 26.12 |
| 3.30 | 6 | 5 1 1 | 25.98 |
| 3.20 | 17 | 3 1 2 | 27.82 |
| 3.09 | 7 | 4 0 2* | 28.84 |
| 3.05 | 15 | 0 2 2 | 29.24 |
| 3.02 | 30 | 1 2 2 | 29.60 |
| 2.884 | 1 | 6 1 1 | 30.98 |
| 2.815 | 6 | 2 3 1 | 31.76 |
| 2.766 | 4 | 3 2 2 | 32.34 |
| 2.693 | 3 | 6 2 0 | 33.24 |
| 2.687 | 3 | 5 1 2 | 33.32 |
| 2.657 | 2 | 4 3 0 | 33.70 |
| 2.592 | 6 | 4 2 2 | 34.58 |
| 2.539 | 4 | 1 1 3 | 35.32 |
| 2.532 | 4 | 6 0 2 | 35.42 |
| 2.478 | 3 | 2 1 3 | 36.22 |
| 2.445 | 1 | 6 1 2 | 36.72 |
| 2.410 | 2 | 5 2 2 | 37.28 |
| 2.377 | 5 | 8 1 0 | 37.82 |
| 2.353 | 1 | 5 3 1 | 38.22 |
| 2.311 | 3 | 7 2 1* | 38.94 |
| 2.304 | 4 | 1 2 3 | 39.06 |
| 2.295 | 5 | 7 0 2 | 39.22 |
| 2.273 | 6 | 6 3 0* | 39.62 |
| 2.258 | 2 | 2 2 3* | 39.90 |
| 2.214 | 2 | 2 4 1 | 40.72 |
| 2.186 | 4 | 3 2 3* | 41.26 |
| 2.097 | 1 | 4 2 3 | 43.10 |
| 2.065 | 2 | 7 2 2 | 43.80 |
| 2.055 | 2 | 9 1 1 | 44.02 |
| 2.024 | 2 | 1 3 3 | 44.74 |
| 1.967 | 1 | 5 4 1* | 46.12 |
| 1.943 | 3 | 3 3 3* | 46.72 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.919 | 3 | 6 | 4 | 0+ | 47.32 |
| 1.915 | 3 | 9 | 0 | 2+ | 47.44 |
| 1.892 | 2 | 7 | 1 | 3+ | 48.06 |
| 1.884 | 2 | 8 | 3 | 1+ | 48.28 |
| 1.880 | 2 | 4 | 3 | 3+ | 48.38 |
| 1.870 | 3 | 10 | 1 | 1+ | 48.64 |
| 1.838 | 1 | 0 | 2 | 4+ | 49.56 |
| 1.813 | 1 | 2 | 5 | 1+ | 50.28 |
| 1.808 | 2 | 2 | 2 | 4+ | 50.44 |
| 1.771 | 4 | 3 | 2 | 4+ | 51.58 |
| 1.748 | 2 | 5 | 1 | 4 | 52.30 |
| 1.744 | 2 | 8 | 3 | 2 | 52.42 |
| 1.708 | 1 | 3 | 4 | 3+ | 53.60 |
| 1.668 | 1 | 10 | 3 | 0 | 55.00 |
| 1.664 | 1 | 2 | 3 | 4+ | 55.16 |
| 1.658 | 1 | 3 | 5 | 2 | 55.38 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 9.82 | 100 | 2 | 0 | 0 | 9.00 |
| 6.82 | 39 | 2 | 1 | 0 | 12.97 |
| 5.83 | 85 | 1 | 1 | 1 | 15.18 |
| 5.18 | 33 | 2 | 1 | 1 | 17.09 |
| 4.91 | 3 | 4 | 0 | 0 | 18.05 |
| 4.74 | 6 | 0 | 2 | 0 | 18.70 |
| 4.47 | 28 | 3 | 1 | 1 | 19.87 |
| 4.36 | 29 | 4 | 1 | 0 | 20.35 |
| 4.27 | 5 | 2 | 2 | 0 | 20.79 |
| 4.08 | 43 | 0 | 2 | 1 | 21.79 |
| 3.99 | 61 | 1 | 2 | 1 | 22.26 |
| 3.99 | 4 | 0 | 0 | 2 | 22.27 |
| 3.91 | 31 | 1 | 0 | 2 | 22.73 |
| 3.83 | 8 | 4 | 1 | 1 | 23.23 |
| 3.76 | 39 | 2 | 2 | 1 | 23.61 |
| 3.70 | 82 | 2 | 0 | 2 | 24.06 |
| 3.61 | 28 | 1 | 1 | 2 | 24.61 |
| 3.46 | 2 | 3 | 2 | 1 | 25.73 |
| 3.44 | 53 | 2 | 1 | 2 | 25.85 |
| 3.41 | 1 | 4 | 2 | 0 | 26.11 |
| 3.41 | 5 | 3 | 0 | 2 | 26.14 |
| 3.30 | 6 | 5 | 1 | 1 | 26.97 |
| 3.21 | 20 | 3 | 1 | 2 | 27.80 |
| 3.10 | 4 | 4 | 0 | 2 | 28.81 |
| 3.09 | 3 | 6 | 1 | 0 | 28.83 |
| 3.05 | 16 | 0 | 2 | 2 | 29.23 |
| 3.02 | 34 | 1 | 2 | 2 | 29.59 |
| 3.01 | 2 | 2 | 3 | 0 | 29.67 |
| 2.885 | 1 | 6 | 1 | 1 | 30.97 |
| 2.828 | 2 | 5 | 2 | 1 | 31.61 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.815 | 6 | 2 | 3 | 1 | 31.76 |
| 2.767 | 4 | 3 | 2 | 2 | 32.33 |
| 2.694 | 3 | 6 | 2 | 0 | 33.23 |
| 2.685 | 1 | 5 | 1 | 2 | 33.35 |
| 2.658 | 2 | 4 | 3 | 0 | 33.69 |
| 2.592 | 8 | 4 | 2 | 2 | 34.57 |
| 2.552 | 1 | 6 | 2 | 1 | 35.13 |
| 2.549 | 1 | 7 | 1 | 1 | 35.17 |
| 2.539 | 4 | 1 | 1 | 3 | 35.32 |
| 2.531 | 3 | 6 | 0 | 2 | 35.44 |
| 2.478 | 3 | 2 | 1 | 3 | 36.22 |
| 2.445 | 1 | 6 | 1 | 2 | 36.73 |
| 2.410 | 2 | 5 | 2 | 2 | 37.27 |
| 2.377 | 5 | 8 | 1 | 0 | 37.82 |
| 2.371 | 1 | 0 | 4 | 0 | 37.92 |
| 2.353 | 1 | 5 | 3 | 1 | 38.22 |
| 2.317 | 1 | 3 | 3 | 2 | 38.83 |
| 2.311 | 2 | 7 | 2 | 1 | 38.94 |
| 2.304 | 2 | 1 | 2 | 3 | 39.07 |
| 2.295 | 5 | 7 | 0 | 2 | 39.22 |
| 2.278 | 1 | 8 | 1 | 1 | 39.53 |
| 2.274 | 4 | 6 | 3 | 0 | 39.60 |
| 2.273 | 2 | 0 | 4 | 1 | 39.63 |
| 2.258 | 1 | 2 | 2 | 3 | 39.90 |
| 2.257 | 1 | 1 | 4 | 1 | 39.90 |
| 2.214 | 3 | 2 | 4 | 1 | 40.72 |
| 2.187 | 2 | 6 | 3 | 1 | 41.25 |
| 2.186 | 3 | 3 | 2 | 3 | 41.26 |
| 2.145 | 1 | 5 | 1 | 3 | 42.09 |
| 2.097 | 1 | 4 | 2 | 3 | 43.09 |
| 2.066 | 3 | 7 | 2 | 2 | 43.79 |
| 2.055 | 2 | 9 | 1 | 1 | 44.03 |
| 2.024 | 3 | 1 | 3 | 3 | 44.73 |
| 1.967 | 1 | 5 | 4 | 1 | 46.11 |
| 1.943 | 2 | 3 | 3 | 3 | 46.70 |
| 1.942 | 2 | 1 | 1 | 4 | 46.73 |
| 1.923 | 1 | 10 | 1 | 0 | 47.22 |
| 1.920 | 2 | 6 | 4 | 0 | 47.30 |
| 1.915 | 1 | 9 | 0 | 2 | 47.45 |
| 1.893 | 1 | 6 | 2 | 3 | 48.03 |
| 1.891 | 2 | 7 | 1 | 3 | 48.06 |
| 1.884 | 1 | 8 | 3 | 1 | 48.26 |
| 1.880 | 1 | 4 | 3 | 3 | 48.38 |
| 1.877 | 1 | 9 | 1 | 2 | 48.47 |
| 1.871 | 1 | 3 | 1 | 4 | 48.63 |
| 1.870 | 2 | 10 | 1 | 1 | 48.66 |
| 1.839 | 1 | 0 | 2 | 4 | 49.54 |
| 1.813 | 1 | 2 | 5 | 1 | 50.27 |
| 1.807 | 1 | 2 | 2 | 4 | 50.46 |
| 1.776 | 1 | 3 | 5 | 1 | 51.41 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.772 | 2 | 8 | 1 | 3 | 51.53 |
| 1.770 | 3 | 3 | 2 | 4 | 51.59 |
| 1.763 | 1 | 1 | 4 | 3 | 51.83 |
| 1.748 | 2 | 5 | 1 | 4 | 52.29 |
| 1.744 | 1 | 8 | 3 | 2 | 52.43 |
| 1.722 | 1 | 4 | 2 | 4 | 53.15 |
| 1.708 | 2 | 3 | 4 | 3 | 53.60 |
| 1.668 | 1 | 10 | 3 | 0 | 55.00 |
| 1.663 | 1 | 2 | 3 | 4 | 55.20 |
| 1.657 | 1 | 3 | 5 | 2 | 55.40 |
| 1.633 | 1 | 10 | 3 | 1 | 56.29 |

# Allobarbital, $C_{10}H_{12}N_2O_3$

Synonyms
5,5 - diallylbarbituric acid, Dial

Structure
Monoclinic, C2/c (15), Z = 8. The structure was determined by Escobar [1975].

Atom positions
There was some disorder in the structure, with one carbon randomly occupying 2 sites in the proportion of 4 to 1. All other atoms were in general positions [ibid.].

Lattice constants
a = 14.570 Å
b = 7.289
c = 20.618
β = 99.83°
(published values: a = 14.569(6), b = 7.289(4), c = 20.617(7), β = 99.83(4)° [Escobar, 1975]).

CD cell: a = 20.618, b = 7.289, c = 14.570, β = 99.83°, space group A2/a; a/b = 2.8286, c/b = 1.9989

Volume
2157.5 Å$^3$

Density
(measured) 1.278
(calculated) 1.282

Thermal parameters
Isotropic: overall B = 4.0

Scattering factors
$C^0$, $H^0$, $N^0$, $O^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.627 \times 10^{-3}$
$I/I_c$ (calculated) = 0.65

Additional pattern
1. PDF card 5-158 [Huang, 1951]

References
Escobar, C. (1975). Acta Crystallogr. B31, 1059.
Huang, T.-Y. (1951). Acta Pharm. Int. 2, 43.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 10.16 | 6 | 0 0 2 | 8.70 |
| 7.17 | 3 | 2 0 0 | 12.34 |
| 6.50 | 100 | 1 1 0 | 13.62 |
| 6.39 | 52 | -2 0 2 | 13.84 |
| 6.05 | 51 | 1 1 1 | 14.62 |
| 5.68 | 16 | -1 1 2 | 15.60 |
| 5.43 | 26 | 2 0 2 | 16.30 |
| 5.29 | 25 | 1 1 2 | 16.76 |
| 5.08 | 44 | 0 0 4 | 17.46 |
| 4.88 | 33 | -1 1 3 | 18.18 |
| 4.52 | 2 | -2 0 4 | 19.62 |
| 4.16 | 6 | -1 1 4 | 21.34 |
| 4.03 | 34 | -3 1 1 | 22.02 |
| 4.00 | 14 | 3 1 0 | 22.20 |
| 3.917 | 3 | -3 1 2 | 22.68 |
| 3.821 | 7 | 3 1 1 | 23.26 |
| 3.681 | 12 | -3 1 3 | 24.16 |
| 3.642 | 22 | 0 2 0 | 24.42 |
| 3.587 | 10 | 0 2 1 | 24.80 |
| 3.553 | 6 | 3 1 2 | 25.04 |
| 3.386 | 6 | -3 1 4 | 26.30 |
| 3.329 | 4 | 1 1 5 | 26.76 |
| 3.285 | 14 | -2 0 6 | 27.12 |
| 3.248 | 52 | 2 2 0* | 27.44 |
| 3.216 | 15 | 4 0 2* | 27.72 |
| 3.169 | 5 | 2 2 1* | 28.14 |
| 3.102 | 6 | -1 1 6 | 28.76 |
| 3.026 | 11 | 2 2 2* | 29.50 |
| 2.944 | 18 | 3 1 4 | 30.34 |
| 2.877 | 2 | 2 0 6 | 31.06 |
| 2.845 | 2 | 2 2 3 | 31.42 |
| 2.788 | 2 | -3 1 6 | 32.08 |
| 2.714 | 9 | 4 0 4* | 32.98 |
| 2.692 | 4 | -5 1 2 | 33.26 |
| 2.671 | 3 | 5 1 0 | 33.52 |
| 2.639 | 6 | -2 2 5* | 33.94 |
| 2.595 | 1 | 5 1 1 | 34.54 |
| 2.555 | 4 | -4 2 2 | 35.10 |
| 2.534 | 5 | -2 0 8 | 35.40 |
| 2.481 | 2 | 0 2 6 | 36.18 |
| 2.447 | 3 | 2 2 5 | 36.70 |
| 2.429 | 5 | -1 1 8 | 36.98 |
| 2.420 | 5 | 3 1 6 | 37.12 |
| 2.405 | 3 | -4 2 4 | 37.36 |
| 2.399 | 3 | 1 3 0 | 37.46 |
| 2.388 | 3 | -1 3 1 | 37.64 |
| 2.371 | 4 | 1 3 1 | 37.92 |
| 2.346 | 3 | -1 3 2 | 38.34 |
| 2.323 | 2 | -6 0 4 | 38.74 |
| 2.317 | 2 | 1 3 2 | 38.84 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.275 | 1 | 2 | 0 | 8* | 39.58 |
| 2.245 | 1 | 6 | 0 | 2 | 40.14 |
| 2.223 | 2 | 5 | 1 | 4 | 40.54 |
| 2.184 | 2 | -1 | 1 | 9 | 41.30 |
| 2.179 | 2 | 4 | 2 | 4 | 41.40 |
| 2.172 | 4 | -3 | 3 | 1 | 41.54 |
| 2.167 | 4 | 3 | 3 | 0 | 41.64 |
| 2.082 | 2 | 1 | 1 | 9* | 43.42 |
| 2.046 | 2 | -4 | 2 | 7 | 44.24 |
| 2.033 | 1 | 0 | 0 | 10* | 44.54 |
| 2.006 | 1 | -5 | 1 | 8 | 45.16 |
| 2.000 | 2 | -6 | 2 | 3* | 45.30 |
| 1.984 | 1 | -7 | 1 | 3* | 45.68 |
| 1.959 | 1 | -6 | 2 | 4 | 46.32 |
| 1.952 | 1 | -7 | 1 | 4* | 46.48 |
| 1.923 | 1 | -4 | 2 | 8* | 47.22 |
| 1.913 | 1 | -4 | 0 | 10* | 47.48 |
| 1.861 | 1 | -5 | 3 | 2 | 48.90 |
| 1.853 | 1 | 3 | 3 | 5* | 49.12 |
| 1.848 | 1 | 6 | 2 | 3 | 49.26 |
| 1.843 | 1 | -7 | 1 | 6 | 49.42 |
| 1.822 | 1 | 1 | 3 | 7* | 50.02 |
| 1.813 | 1 | 4 | 2 | 7* | 50.30 |
| 1.791 | 2 | -8 | 0 | 4* | 50.96 |
| 1.766 | 2 | 2 | 4 | 0 | 51.72 |
| 1.746 | 1 | 7 | 1 | 4 | 52.36 |
| 1.714 | 1 | -2 | 0 | 12* | 53.40 |
| 1.710 | 1 | -8 | 0 | 6* | 53.54 |
| 1.690 | 1 | -2 | 4 | 4* | 54.22 |
| 1.683 | 1 | 5 | 3 | 4 | 54.46 |
| 1.630 | 1 | -4 | 4 | 1* | 56.42 |
| 1.624 | 2 | -4 | 4 | 2* | 56.62 |
| 1.608 | 1 | -4 | 4 | 3* | 57.24 |
| 1.595 | 1 | 2 | 4 | 5* | 57.76 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 10.16 | 6 | 0 | 0 | 2 | 8.70 |
| 7.18 | 3 | 2 | 0 | 0 | 12.32 |
| 6.50 | 100 | 1 | 1 | 0 | 13.61 |
| 6.40 | 45 | -2 | 0 | 2 | 13.83 |
| 6.33 | 4 | -1 | 1 | 1 | 13.97 |
| 6.06 | 53 | 1 | 1 | 1 | 14.62 |
| 5.68 | 16 | -1 | 1 | 2 | 15.60 |
| 5.44 | 27 | 2 | 0 | 2 | 16.28 |
| 5.29 | 26 | 1 | 1 | 2 | 16.74 |
| 5.08 | 47 | 0 | 0 | 4 | 17.45 |
| 4.88 | 36 | -1 | 1 | 3 | 18.16 |
| 4.53 | 3 | -2 | 0 | 4 | 19.60 |
| 4.16 | 6 | -1 | 1 | 4 | 21.34 |
| 4.04 | 37 | -3 | 1 | 1 | 22.01 |
| 4.00 | 11 | 3 | 1 | 0 | 22.21 |
| 3.917 | 3 | -3 | 1 | 2 | 22.68 |
| 3.823 | 8 | 3 | 1 | 1 | 23.25 |
| 3.682 | 12 | -3 | 1 | 3 | 24.15 |
| 3.645 | 25 | 0 | 2 | 0 | 24.40 |
| 3.587 | 11 | 0 | 2 | 1 | 24.80 |
| 3.553 | 6 | 3 | 1 | 2 | 25.04 |
| 3.386 | 6 | -3 | 1 | 4 | 26.30 |
| 3.331 | 3 | 1 | 1 | 5 | 26.74 |
| 3.286 | 14 | -2 | 0 | 6 | 27.11 |
| 3.250 | 37 | 2 | 2 | 0 | 27.42 |
| 3.248 | 33 | -2 | 2 | 1 | 27.44 |
| 3.247 | 1 | 3 | 1 | 3 | 27.45 |
| 3.216 | 13 | 4 | 0 | 2 | 27.72 |
| 3.209 | 3 | 0 | 2 | 3 | 27.78 |
| 3.171 | 3 | 2 | 2 | 1 | 28.12 |
| 3.167 | 1 | -2 | 2 | 2 | 28.16 |
| 3.103 | 7 | -1 | 1 | 6 | 28.75 |
| 3.028 | 10 | 2 | 2 | 2 | 29.48 |
| 3.022 | 4 | -2 | 2 | 3 | 29.53 |
| 2.961 | 7 | 0 | 2 | 4 | 30.16 |
| 2.945 | 21 | 3 | 1 | 4 | 30.33 |
| 2.878 | 3 | 2 | 0 | 6 | 31.04 |
| 2.845 | 2 | 2 | 2 | 3 | 31.42 |
| 2.788 | 2 | -3 | 1 | 6 | 32.08 |
| 2.730 | 1 | -1 | 1 | 7 | 32.78 |
| 2.720 | 7 | 4 | 0 | 4 | 32.90 |
| 2.713 | 5 | 0 | 2 | 5 | 32.99 |
| 2.705 | 1 | -5 | 1 | 1 | 33.10 |
| 2.704 | 1 | -4 | 0 | 6 | 33.10 |
| 2.691 | 3 | -5 | 1 | 2 | 33.27 |
| 2.671 | 2 | 5 | 1 | 0 | 33.52 |
| 2.646 | 2 | 2 | 2 | 4 | 33.85 |
| 2.639 | 5 | -2 | 2 | 5 | 33.94 |
| 2.596 | 1 | 5 | 1 | 1 | 34.53 |
| 2.554 | 5 | -4 | 2 | 2 | 35.10 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.534 | 6 | -2 | 0 | 8 | 35.40 |
| 2.481 | 2 | 0 | 2 | 6 | 36.18 |
| 2.447 | 3 | 2 | 2 | 5 | 36.69 |
| 2.430 | 5 | -1 | 1 | 8 | 36.97 |
| 2.420 | 4 | 3 | 1 | 6 | 37.13 |
| 2.404 | 3 | -4 | 2 | 4 | 37.37 |
| 2.396 | 1 | 1 | 3 | 0 | 37.51 |
| 2.387 | 2 | -1 | 3 | 1 | 37.65 |
| 2.371 | 4 | 1 | 3 | 1 | 37.91 |
| 2.347 | 3 | -1 | 3 | 2 | 38.33 |
| 2.323 | 2 | -6 | 0 | 4 | 38.74 |
| 2.317 | 1 | 1 | 3 | 2 | 38.84 |
| 2.275 | 1 | 2 | 0 | 8 | 39.58 |
| 2.245 | 1 | 6 | 0 | 2 | 40.14 |
| 2.223 | 2 | 5 | 1 | 4 | 40.55 |
| 2.185 | 2 | -1 | 1 | 9 | 41.28 |
| 2.180 | 1 | 4 | 2 | 4 | 41.39 |
| 2.172 | 5 | -3 | 3 | 1 | 41.54 |
| 2.166 | 1 | 3 | 3 | 0 | 41.66 |
| 2.083 | 1 | 1 | 1 | 9 | 43.41 |
| 2.080 | 1 | -2 | 2 | 8 | 43.46 |
| 2.046 | 2 | -4 | 2 | 7 | 44.23 |
| 2.031 | 1 | 0 | 0 | 10 | 44.57 |
| 2.006 | 1 | -5 | 1 | 8 | 45.15 |
| 2.000 | 1 | 6 | 2 | 0 | 45.30 |
| 1.997 | 1 | -6 | 2 | 3 | 45.37 |
| 1.985 | 1 | -7 | 1 | 3 | 45.67 |
| 1.959 | 1 | -6 | 2 | 4 | 46.32 |
| 1.923 | 1 | -4 | 2 | 8 | 47.24 |
| 1.861 | 1 | -5 | 3 | 2 | 48.90 |
| 1.848 | 1 | 6 | 2 | 3 | 49.27 |
| 1.842 | 1 | -7 | 1 | 6 | 49.43 |
| 1.826 | 1 | 5 | 1 | 7 | 49.90 |
| 1.791 | 2 | -8 | 0 | 4 | 50.96 |
| 1.766 | 2 | 2 | 4 | 0 | 51.71 |
| 1.746 | 1 | 7 | 1 | 4 | 52.37 |
| 1.714 | 1 | -2 | 0 | 12 | 53.40 |
| 1.690 | 1 | -2 | 4 | 4 | 54.22 |
| 1.683 | 1 | 5 | 3 | 4 | 54.47 |
| 1.670 | 1 | -1 | 1 | 12 | 54.94 |
| 1.630 | 1 | -4 | 4 | 1 | 56.42 |
| 1.624 | 1 | -4 | 4 | 2 | 56.63 |
| 1.608 | 1 | -4 | 4 | 3 | 57.23 |
| 1.595 | 1 | 2 | 4 | 5 | 57.74 |

# Calcium carbonate, aragonite, $CaCO_3$

Structure
Orthorhombic, Pnma (62), Z = 4. The structure was determined by Bragg [1924] and refined by de Villiers [1971]. Aragonite is isostructural with strontianite ($SrCO_3$) and witherite ($BaCO_3$) [de Villiers, 1971].

Atom positions
4(c) 4 calcium
4(c) 4 carbon
4(c) 4 oxygen(1)
8(d) 8 oxygen(2)

Polymorphism
There are 2 hexagonal polymorphs, calcite and vaterite; the 3 forms may coexist in synthetic samples.

Lattice constants
a = 5.740(1)
b = 4.9614(6)
c = 7.966(1)
This cell was refined from NBS data [Swanson, Fuyat and Ugrinic, 1954, and on PDF card 5-453]

CD cell: a=5.740(1), b=7.966(1), c=4.9614(6), space group, Pnam, a/b = 0.7206, c/b = 0.6228

Volume
226.9 $Å^3$

Density
(calculated) 2.931 $g/cm^3$

Thermal parameters
Anisotropic [de Villiers, 1971]

Scattering factors
$Ca^{2+}$, $C^0$ [International Tables, 1962]
$O^{2-}$ [Suzuki, 1960]

Scale factors (integrated intensities)
$\gamma = 0.220 \times 10^{-3}$
$I/I_c$ (calculated) = 0.98

Additional patterns
1. PDF card 5-453 [Powder Diffraction Data 1976]
2. PDF card 24-25 [Smith et al., 1973]

References

Bragg, W. L. (1924). Proc. Roy. Soc. A105, 16.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.
Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081), p. 16.
Smith, D. K. et al. (1973). The Annual Report to the Joint Committee on Powder Diffraction Standards.
Suzuki, T. (1960). Acta Crystallogr. 13, 279.
Swanson, H. E., Fuyat, R. K, and Ugrinic, G. M. (1954). Nat'l Bur. Std. U.S. Circ. 539, 3, 53.
de Villiers, J. P. R. (1971). Am. Mineralogist 56, 758.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.653 | 1 | 1 0 1 | 19.06 |
| 4.211 | 5 | 0 1 1 | 21.08 |
| 3.980 | 2 | 0 0 2 | 22.32 |
| 3.394 | 100 | 1 1 1 | 26.24 |
| 3.271 | 62 | 1 0 2 | 27.24 |
| 2.8698 | 4 | 2 0 0 | 31.14 |
| 2.7315 | 11 | 1 1 2 | 32.76 |
| 2.6995 | 62 | 2 0 1 | 33.16 |
| 2.4821 | 43 | 2 1 0+ | 36.16 |
| 2.4100 | 18 | 1 0 3 | 37.28 |
| 2.3708 | 42 | 2 1 1 | 37.92 |
| 2.3411 | 31 | 0 1 3 | 38.42 |
| 2.3283 | 24 | 2 0 2 | 38.64 |
| 2.1893 | 15 | 1 2 1 | 41.20 |
| 2.1682 | 1 | 1 1 3 | 41.62 |
| 2.1055 | 22 | 0 2 2 | 42.92 |
| 1.9911 | 6 | 0 0 4 | 45.52 |
| 1.9771 | 69 | 1 2 2 | 45.86 |
| 1.9498 | 1 | 2 0 3 | 46.54 |
| 1.8813 | 34 | 1 0 4 | 48.34 |
| 1.8769 | 38 | 2 2 0 | 48.46 |
| 1.8268 | 3 | 2 2 1 | 49.88 |
| 1.8139 | 28 | 2 1 3 | 50.26 |
| 1.7591 | 4 | 1 1 4 | 51.94 |
| 1.7416 | 28 | 3 1 1 | 52.50 |
| 1.7282 | 11 | 1 2 3 | 52.94 |
| 1.7246 | 18 | 3 0 2 | 53.06 |
| 1.6979 | 2 | 2 2 2 | 53.96 |
| 1.6359 | 2 | 2 0 4 | 56.18 |
| 1.6296 | 1 | 3 1 2 | 56.42 |
| 1.6190 | 2 | 0 3 1 | 56.82 |
| 1.5585 | 6 | 1 3 1 | 59.24 |
| 1.5350 | 2 | 1 0 5 | 60.24 |
| 1.5318 | 1 | 2 2 3 | 60.38 |
| 1.5168 | 1 | 0 1 5 | 61.04 |
| 1.4991 | 6 | 1 2 4 | 61.84 |
| 1.4759 | 3 | 1 3 2 | 62.92 |
| 1.4663 | 7 | 1 1 5 | 63.38 |
| 1.4329 | 1 | 2 3 0+ | 65.04 |
| 1.4121 | 4 | 4 0 1 | 66.12 |
| 1.4102 | 4 | 2 3 1 | 66.22 |
| 1.4038 | 4 | 0 3 3 | 66.56 |
| 1.3786 | 1 | 4 1 0 | 67.94 |
| 1.3659 | 4 | 2 2 4 | 68.66 |
| 1.3583 | 5 | 4 1 1 | 69.10 |
| 1.3501 | 2 | 4 0 2 | 69.58 |
| 1.3410 | 3 | 2 1 5 | 70.12 |
| 1.3278 | 2 | 0 0 6 | 70.92 |
| 1.3055 | 1 | 1 2 5 | 72.32 |
| 1.3024 | 1 | 4 1 2 | 72.52 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.2611 | 6 | 2 | 3 | 3 | 75.30 |
| 1.2404 | 7 | 0 | 4 | 0+ | 76.78 |
| 1.2360 | 9 | 3 | 3 | 1 | 77.10 |
| 1.2235 | 6 | 4 | 1 | 3 | 78.04 |
| 1.2146 | 2 | 2 | 2 | 5 | 78.72 |
| 1.2057 | 8 | 3 | 2 | 4+ | 79.42 |
| 1.1937 | 1 | 3 | 3 | 2 | 80.38 |
| 1.1888 | 6 | 3 | 1 | 5 | 80.78 |
| 1.1706 | 9 | 0 | 2 | 6 | 82.30 |
| 1.1643 | 1 | 4 | 0 | 4 | 82.84 |
| 1.1598 | 3 | 1 | 4 | 2 | 83.24 |
| 1.1470 | 1 | 1 | 2 | 6 | 84.38 |
| 1.1385 | 1 | 2 | 4 | 0 | 85.16 |
| 1.1359 | 1 | 5 | 0 | 1 | 85.40 |
| 1.1333 | 1 | 4 | 1 | 4 | 85.64 |
| 1.1318 | 1 | 3 | 3 | 3 | 85.78 |
| 1.1269 | 2 | 2 | 4 | 1 | 86.24 |
| 1.1251 | 4 | 1 | 3 | 5 | 86.42 |
| 1.1164 | 1 | 1 | 0 | 7 | 87.26 |
| 1.1075 | 2 | 5 | 1 | 1 | 88.14 |
| 1.1031 | 1 | 5 | 0 | 2+ | 88.58 |
| 1.0978 | 1 | 3 | 2 | 5 | 89.12 |
| 1.0947 | 2 | 2 | 4 | 2 | 89.44 |
| 1.0890 | 1 | 1 | 1 | 7 | 90.04 |
| 1.0839 | 1 | 2 | 2 | 6 | 90.58 |
| 1.0739 | 1 | 4 | 3 | 1 | 91.66 |
| 1.0655 | 2 | 2 | 3 | 5 | 92.60 |
| 1.0595 | 1 | 3 | 3 | 4 | 93.28 |
| 1.0579 | 1 | 2 | 0 | 7 | 93.46 |
| 1.0539 | 1 | 4 | 2 | 4+ | 93.92 |
| 1.0465 | 1 | 2 | 4 | 3 | 94.80 |
| 1.0425 | 1 | 4 | 1 | 5 | 95.28 |
| 1.0356 | 4 | 1 | 4 | 4+ | 96.12 |
| 1.0330 | 4 | 5 | 2 | 1 | 96.44 |
| 1.0180 | 1 | 1 | 2 | 7+ | 98.34 |
| 1.0079 | 4 | 5 | 2 | 2 | 99.68 |
| 1.0070 | 3 | 3 | 4 | 2 | 99.80 |
| 1.0035 | 4 | 4 | 3 | 3 | 100.28 |
| .9986 | 1 | 3 | 2 | 6 | 100.96 |
| .9957 | 1 | 0 | 0 | 8 | 101.36 |
| .9946 | 1 | 5 | 0 | 4 | 101.52 |
| .9884 | 1 | 2 | 4 | 4 | 102.40 |
| .9840 | 2 | 3 | 3 | 5 | 103.04 |
| .9811 | 2 | 1 | 0 | 8 | 103.46 |
| .9795 | 1 | 4 | 2 | 5 | 103.70 |
| .9739 | 2 | 2 | 3 | 6+ | 104.54 |
| .9732 | 1 | 2 | 2 | 7 | 104.66 |
| .9706 | 2 | 1 | 5 | 1 | 105.06 |
| .9648 | 1 | 1 | 4 | 5 | 105.96 |
| .9624 | 1 | 1 | 1 | 8 | 106.34 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .9596 | 3 | 3 | 1 | 7 | 106.78 |
| .9568 | 3 | 6 | 0 | 0 | 107.24 |
| .9520 | 1 | 4 | 3 | 4 | 108.02 |
| .9497 | 1 | 6 | 0 | 1 | 108.40 |
| .9407 | 1 | 2 | 0 | 8 | 109.94 |
| .9378 | 1 | 2 | 5 | 0 | 110.44 |
| .9365 | 1 | 5 | 3 | 1 | 110.68 |
| .9315 | 3 | 2 | 5 | 1+ | 111.58 |
| .9295 | 3 | 0 | 5 | 3 | 111.94 |
| .9252 | 1 | 1 | 3 | 7 | 112.72 |
| .9231 | 1 | 5 | 2 | 4 | 113.12 |
| .9175 | 1 | 1 | 5 | 3+ | 114.18 |
| .9154 | 2 | 5 | 1 | 5 | 114.60 |
| .9132 | 2 | 4 | 4 | 2 | 115.02 |
| .9123 | 3 | 1 | 2 | 8 | 115.20 |
| .9063 | 2 | 0 | 4 | 6+ | 116.40 |
| .9001 | 1 | 6 | 0 | 3 | 117.70 |
| .8961 | 1 | 4 | 3 | 5 | 118.54 |
| .8926 | 1 | 6 | 2 | 0 | 119.30 |
| .8912 | 2 | 2 | 3 | 7 | 119.62 |
| .8856 | 2 | 6 | 1 | 3 | 120.88 |
| .8843 | 2 | 2 | 5 | 3 | 121.18 |
| .8796 | 1 | 2 | 2 | 8 | 122.26 |
| .8776 | 2 | 4 | 1 | 7+ | 122.74 |
| .8755 | 2 | 3 | 5 | 1 | 123.24 |
| .8712 | 1 | 0 | 1 | 9+ | 124.30 |
| .8643 | 2 | 2 | 4 | 6 | 126.06 |
| .8601 | 1 | 3 | 5 | 2 | 127.16 |
| .8523 | 1 | 5 | 3 | 4 | 129.32 |
| .8489 | 1 | 4 | 4 | 4 | 130.30 |
| .8460 | 1 | 6 | 2 | 3 | 131.14 |
| .8439 | 1 | 1 | 3 | 8 | 131.78 |
| .8419 | 3 | 3 | 3 | 7 | 132.40 |
| .8391 | 1 | 4 | 2 | 7 | 133.26 |
| .8378 | 1 | 5 | 4 | 1 | 133.68 |
| .8360 | 1 | 3 | 5 | 3 | 134.26 |
| .8338 | 3 | 2 | 1 | 9+ | 135.00 |
| .8320 | 2 | 3 | 2 | 8 | 135.58 |
| .8269 | 1 | 0 | 6 | 0 | 137.36 |
| .8243 | 1 | 5 | 4 | 2 | 138.30 |
| .8202 | 1 | 6 | 0 | 5 | 139.84 |
| .8161 | 1 | 4 | 5 | 0 | 141.42 |
| .8157 | 1 | 7 | 0 | 1 | 141.58 |
| .8142 | 1 | 6 | 2 | 4+ | 142.20 |
| .8118 | 2 | 4 | 5 | 1 | 143.20 |
| .8116 | 2 | 5 | 3 | 5 | 143.28 |
| .8096 | 2 | 0 | 6 | 2 | 144.14 |
| .8082 | 1 | 2 | 5 | 5+ | 144.76 |
| .8049 | 1 | 7 | 1 | 1 | 146.28 |
| .8031 | 1 | 7 | 0 | 2+ | 147.14 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .8017 | 3 | 1 | 6 | 2 | 147.82 |
| .8006 | 1 | 2 | 2 | 9 | 148.38 |
| .7977 | 1 | 5 | 1 | 7 | 149.90 |
| .7966 | 1 | 0 | 0 | 10 | 150.46 |
| .7946 | 1 | 2 | 6 | 0 | 151.60 |
| .7927 | 1 | 7 | 1 | 2 | 152.70 |
| .7906 | 2 | 6 | 3 | 3 | 154.00 |
| .7890 | 1 | 1 | 0 | 10 | 155.00 |
| .7849 | 2 | 4 | 3 | 7 | 157.90 |
| .7834 | 1 | 7 | 0 | 3 | 159.00 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 4.657 | 1 | 1 | 0 | 1 | 19.04 |
| 4.211 | 5 | 0 | 1 | 1 | 21.08 |
| 3.983 | 2 | 0 | 0 | 2 | 22.30 |
| 3.395 | 100 | 1 | 1 | 1 | 26.22 |
| 3.272 | 62 | 1 | 0 | 2 | 27.23 |
| 2.8700 | 4 | 2 | 0 | 0 | 31.14 |
| 2.7317 | 10 | 1 | 1 | 2 | 32.76 |
| 2.7001 | 65 | 2 | 0 | 1 | 33.15 |
| 2.4843 | 34 | 2 | 1 | 0 | 36.13 |
| 2.4807 | 18 | 0 | 2 | 0 | 36.18 |
| 2.4100 | 18 | 1 | 0 | 3 | 37.28 |
| 2.3716 | 45 | 2 | 1 | 1 | 37.91 |
| 2.3411 | 31 | 0 | 1 | 3 | 38.42 |
| 2.3285 | 21 | 2 | 0 | 2 | 38.64 |
| 2.1894 | 16 | 1 | 2 | 1 | 41.20 |
| 2.1678 | 1 | 1 | 1 | 3 | 41.63 |
| 2.1057 | 24 | 0 | 2 | 2 | 42.92 |
| 1.9915 | 4 | 0 | 0 | 4 | 45.51 |
| 1.9769 | 79 | 1 | 2 | 2 | 45.87 |
| 1.9491 | 1 | 2 | 0 | 3 | 46.56 |
| 1.8815 | 34 | 1 | 0 | 4 | 48.34 |
| 1.8768 | 21 | 2 | 2 | 0 | 48.46 |
| 1.8604 | 1 | 3 | 0 | 1 | 48.92 |
| 1.8268 | 2 | 2 | 2 | 1 | 49.88 |
| 1.8141 | 32 | 2 | 1 | 3 | 50.25 |
| 1.7592 | 4 | 1 | 1 | 4 | 51.94 |
| 1.7420 | 33 | 3 | 1 | 1 | 52.49 |
| 1.7286 | 8 | 1 | 2 | 3 | 52.93 |
| 1.7247 | 15 | 3 | 0 | 2 | 53.06 |
| 1.6977 | 3 | 2 | 2 | 2 | 53.96 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.6362 | 3 | 2 | 0 | 4 | 56.17 |
| 1.6290 | 1 | 3 | 1 | 2 | 56.44 |
| 1.6193 | 2 | 0 | 3 | 1 | 56.81 |
| 1.5584 | 7 | 1 | 3 | 1 | 59.24 |
| 1.5530 | 1 | 0 | 2 | 4 | 59.47 |
| 1.5352 | 2 | 1 | 0 | 5 | 60.23 |
| 1.5326 | 1 | 2 | 2 | 3 | 60.35 |
| 1.5169 | 1 | 0 | 1 | 5 | 61.04 |
| 1.4991 | 7 | 1 | 2 | 4 | 61.84 |
| 1.4884 | 1 | 3 | 2 | 1 | 62.34 |
| 1.4760 | 4 | 1 | 3 | 2 | 62.92 |
| 1.4666 | 8 | 1 | 1 | 5 | 63.37 |
| 1.4350 | 1 | 4 | 0 | 0 | 64.93 |
| 1.4329 | 1 | 2 | 3 | 0 | 65.04 |
| 1.4161 | 1 | 3 | 2 | 2 | 65.91 |
| 1.4123 | 4 | 4 | 0 | 1 | 66.11 |
| 1.4103 | 3 | 2 | 3 | 1 | 66.21 |
| 1.4038 | 4 | 0 | 3 | 3 | 66.56 |
| 1.3785 | 1 | 4 | 1 | 0 | 67.95 |
| 1.3658 | 4 | 2 | 2 | 4 | 68.66 |
| 1.3636 | 1 | 1 | 3 | 3 | 68.79 |
| 1.3583 | 6 | 4 | 1 | 1 | 69.10 |
| 1.3501 | 2 | 4 | 0 | 2 | 69.58 |
| 1.3483 | 1 | 2 | 3 | 2 | 69.68 |
| 1.3411 | 3 | 2 | 1 | 5 | 70.11 |
| 1.3293 | 1 | 3 | 1 | 4 | 70.83 |
| 1.3277 | 2 | 0 | 0 | 6 | 70.93 |
| 1.3054 | 1 | 1 | 2 | 5 | 72.33 |
| 1.3027 | 1 | 4 | 1 | 2 | 72.50 |
| 1.2610 | 8 | 2 | 3 | 3 | 75.30 |
| 1.2421 | 3 | 4 | 2 | 0 | 76.65 |
| 1.2403 | 7 | 0 | 4 | 0 | 76.78 |
| 1.2360 | 10 | 3 | 3 | 1 | 77.10 |
| 1.2235 | 7 | 4 | 1 | 3 | 78.04 |
| 1.2146 | 2 | 2 | 2 | 5 | 78.72 |
| 1.2058 | 9 | 3 | 2 | 4 | 79.41 |
| 1.2050 | 4 | 2 | 0 | 6 | 79.47 |
| 1.1937 | 1 | 3 | 3 | 2 | 80.38 |
| 1.1887 | 7 | 3 | 1 | 5 | 80.79 |
| 1.1858 | 1 | 4 | 2 | 2 | 81.02 |
| 1.1709 | 1 | 2 | 1 | 6 | 82.27 |
| 1.1706 | 11 | 0 | 2 | 6 | 82.30 |
| 1.1642 | 1 | 4 | 0 | 4 | 82.85 |
| 1.1598 | 4 | 1 | 4 | 2 | 83.23 |
| 1.1470 | 1 | 1 | 2 | 6 | 84.38 |
| 1.1386 | 1 | 2 | 4 | 0 | 85.15 |
| 1.1363 | 1 | 5 | 0 | 1 | 85.36 |
| 1.1335 | 1 | 4 | 1 | 4 | 85.63 |
| 1.1318 | 1 | 3 | 3 | 3 | 85.78 |
| 1.1271 | 2 | 2 | 4 | 1 | 86.22 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.1251 | 4 | 1 | 3 | 5 | 86.41 |
| 1.1251 | 1 | 4 | 2 | 3 | 86.41 |
| 1.1163 | 1 | 1 | 0 | 7 | 87.27 |
| 1.1092 | 1 | 0 | 1 | 7 | 87.97 |
| 1.1076 | 3 | 5 | 1 | 1 | 88.13 |
| 1.1031 | 1 | 5 | 0 | 2 | 88.58 |
| 1.1029 | 1 | 1 | 4 | 3 | 88.61 |
| 1.0979 | 1 | 3 | 2 | 5 | 89.11 |
| 1.0947 | 2 | 2 | 4 | 2 | 89.44 |
| 1.0890 | 2 | 1 | 1 | 7 | 90.03 |
| 1.0839 | 2 | 2 | 2 | 6 | 90.58 |
| 1.0740 | 1 | 4 | 3 | 1 | 91.66 |
| 1.0654 | 2 | 2 | 3 | 5 | 92.61 |
| 1.0594 | 1 | 3 | 3 | 4 | 93.28 |
| 1.0579 | 1 | 2 | 0 | 7 | 93.46 |
| 1.0539 | 1 | 4 | 2 | 4 | 93.92 |
| 1.0537 | 1 | 5 | 0 | 3 | 93.94 |
| 1.0528 | 1 | 0 | 4 | 4 | 94.05 |
| 1.0464 | 1 | 2 | 4 | 3 | 94.80 |
| 1.0425 | 2 | 4 | 1 | 5 | 95.28 |
| 1.0356 | 5 | 1 | 4 | 4 | 96.12 |
| 1.0346 | 2 | 2 | 1 | 7 | 96.24 |
| 1.0330 | 2 | 5 | 2 | 1 | 96.43 |
| 1.0189 | 1 | 1 | 3 | 6 | 98.23 |
| 1.0180 | 1 | 1 | 2 | 7 | 98.35 |
| 1.0079 | 4 | 5 | 2 | 2 | 99.68 |
| 1.0070 | 3 | 3 | 4 | 2 | 99.81 |
| 1.0035 | 4 | 4 | 3 | 3 | 100.28 |
| .9985 | 1 | 3 | 2 | 6 | 100.97 |
| .9957 | 1 | 0 | 0 | 8 | 101.35 |
| .9946 | 2 | 5 | 0 | 4 | 101.52 |
| .9884 | 1 | 2 | 4 | 4 | 102.40 |
| .9840 | 2 | 3 | 3 | 5 | 103.04 |
| .9811 | 2 | 1 | 0 | 8 | 103.47 |
| .9796 | 1 | 4 | 2 | 5 | 103.69 |
| .9745 | 1 | 4 | 0 | 6 | 104.45 |
| .9739 | 2 | 2 | 3 | 6 | 104.55 |
| .9731 | 1 | 2 | 2 | 7 | 104.67 |
| .9705 | 2 | 1 | 5 | 1 | 105.07 |
| .9699 | 1 | 5 | 2 | 3 | 105.17 |
| .9648 | 1 | 1 | 4 | 5 | 105.96 |
| .9625 | 1 | 1 | 1 | 8 | 106.33 |
| .9596 | 5 | 3 | 1 | 7 | 106.78 |
| .9567 | 3 | 6 | 0 | 0 | 107.26 |
| .9520 | 1 | 4 | 3 | 4 | 108.02 |
| .9498 | 1 | 6 | 0 | 1 | 108.38 |
| .9407 | 1 | 2 | 0 | 8 | 109.93 |
| .9384 | 1 | 4 | 4 | 0 | 110.34 |
| .9378 | 1 | 2 | 5 | 0 | 110.45 |
| .9365 | 2 | 5 | 3 | 1 | 110.67 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .9319 | 2 | 4 | 4 | 1 | 111.49 |
| .9314 | 1 | 5 | 0 | 5 | 111.59 |
| .9314 | 2 | 2 | 5 | 1 | 111.59 |
| .9295 | 2 | 0 | 5 | 3 | 111.94 |
| .9252 | 1 | 1 | 3 | 7 | 112.72 |
| .9232 | 1 | 5 | 2 | 4 | 113.11 |
| .9224 | 1 | 3 | 4 | 4 | 113.25 |
| .9175 | 1 | 1 | 5 | 3 | 114.18 |
| .9154 | 2 | 5 | 1 | 5 | 114.59 |
| .9134 | 1 | 4 | 4 | 2 | 114.99 |
| .9128 | 1 | 2 | 5 | 2 | 115.10 |
| .9123 | 4 | 1 | 2 | 8 | 115.20 |
| .9071 | 1 | 4 | 2 | 6 | 116.26 |
| .9064 | 2 | 0 | 4 | 6 | 116.40 |
| .9000 | 1 | 6 | 0 | 3 | 117.71 |
| .8961 | 2 | 4 | 3 | 5 | 118.54 |
| .8926 | 1 | 6 | 2 | 0 | 119.31 |
| .8912 | 2 | 2 | 3 | 7 | 119.63 |
| .8870 | 1 | 6 | 2 | 1 | 120.54 |
| .8856 | 3 | 6 | 1 | 3 | 120.88 |
| .8843 | 3 | 2 | 5 | 3 | 121.17 |
| .8833 | 1 | 3 | 0 | 8 | 121.40 |
| .8796 | 2 | 2 | 2 | 8 | 122.26 |
| .8777 | 1 | 1 | 5 | 4 | 122.72 |
| .8776 | 1 | 4 | 1 | 7 | 122.74 |
| .8755 | 3 | 3 | 5 | 1 | 123.24 |
| .8748 | 1 | 1 | 0 | 9 | 123.42 |
| .8714 | 1 | 0 | 1 | 9 | 124.26 |
| .8710 | 1 | 6 | 2 | 2 | 124.35 |
| .8696 | 1 | 3 | 1 | 8 | 124.70 |
| .8643 | 4 | 2 | 4 | 6 | 126.06 |
| .8623 | 1 | 6 | 0 | 4 | 126.58 |
| .8601 | 1 | 3 | 5 | 2 | 127.17 |
| .8523 | 1 | 5 | 3 | 4 | 129.31 |
| .8496 | 1 | 6 | 1 | 4 | 130.10 |
| .8489 | 1 | 4 | 4 | 4 | 130.31 |
| .8461 | 1 | 6 | 2 | 3 | 131.13 |
| .8458 | 1 | 2 | 0 | 9 | 131.21 |
| .8438 | 1 | 1 | 3 | 8 | 131.82 |
| .8423 | 1 | 0 | 5 | 5 | 132.28 |
| .8419 | 6 | 3 | 3 | 7 | 132.41 |
| .8396 | 1 | 4 | 3 | 6 | 133.11 |
| .8391 | 2 | 4 | 2 | 7 | 133.27 |
| .8378 | 1 | 5 | 4 | 1 | 133.67 |
| .8361 | 1 | 3 | 5 | 3 | 134.25 |
| .8338 | 5 | 2 | 1 | 9 | 135.00 |
| .8334 | 2 | 1 | 5 | 5 | 135.14 |
| .8321 | 3 | 3 | 2 | 8 | 135.55 |
| .8297 | 1 | 1 | 4 | 7 | 136.36 |
| .8281 | 1 | 6 | 3 | 0 | 136.93 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2Θ(°) λ = 1.540598Å |
| .8269 | 1 | 0 | 6 | 0 | 137.36 |
| .8250 | 1 | 1 | 2 | 9 | 138.04 |
| .8243 | 2 | 5 | 4 | 2 | 138.30 |
| .8237 | 1 | 6 | 3 | 1 | 138.53 |
| .8202 | 1 | 6 | 0 | 5 | 139.84 |
| .8162 | 1 | 4 | 5 | 0 | 141.40 |
| .8157 | 1 | 7 | 0 | 1 | 141.59 |
| .8145 | 1 | 6 | 2 | 4 | 142.07 |
| .8142 | 1 | 1 | 6 | 1 | 142.21 |
| .8119 | 4 | 4 | 5 | 1 | 143.15 |
| .8115 | 4 | 5 | 3 | 5 | 143.31 |
| .8096 | 1 | 0 | 6 | 2 | 144.13 |
| .8086 | 1 | 4 | 4 | 5 | 144.61 |
| .8082 | 1 | 5 | 0 | 7 | 144.77 |
| .8082 | 1 | 2 | 5 | 5 | 144.77 |
| .8056 | 1 | 3 | 5 | 4 | 145.96 |
| .8049 | 1 | 2 | 4 | 7 | 146.28 |
| .8049 | 2 | 7 | 1 | 1 | 146.29 |
| .8032 | 2 | 7 | 0 | 2 | 147.11 |
| .8031 | 1 | 5 | 4 | 3 | 147.15 |
| .8017 | 7 | 1 | 6 | 2 | 147.82 |
| .8005 | 1 | 2 | 2 | 9 | 148.40 |
| .7995 | 1 | 4 | 5 | 2 | 148.91 |
| .7977 | 3 | 5 | 1 | 7 | 149.89 |
| .7966 | 1 | 0 | 0 | 10 | 150.47 |
| .7946 | 3 | 2 | 6 | 0 | 151.60 |
| .7930 | 1 | 3 | 1 | 9 | 152.52 |
| .7928 | 1 | 7 | 1 | 2 | 152.61 |
| .7905 | 5 | 6 | 3 | 3 | 154.01 |
| .7890 | 2 | 1 | 0 | 10 | 154.98 |
| .7848 | 5 | 4 | 3 | 7 | 157.90 |
| .7835 | 1 | 7 | 0 | 3 | 158.94 |

# Calcium oxide (lime), CaO

Structure
Cubic, Fm3m (225), Z = 4, isostructural with NaCl [Davey and Hoffman, 1920].

Atom positions
4(a) 4 calcium
4(b) 4 oxygen

Lattice constants
a = 4.8108 Å
(published value, 4.8105 [Swanson and Tatge, 1953, and on PDF card 4-777])

Volume
111.34 $Å^3$

Density
(calculated) 3.345 $g/cm^3$

Thermal parameters
Isotropic: calcium B = 0.5; oxygen B = 1.0

Scattering factors
$O^{2-}$ [Suzuki, 1960]
$Ca^{2+}$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.611 \times 10^{-3}$
$I/I_c$ (calculated) = 4.56

Additional pattern
1. PDF card 4-777 [Powder Diffraction Data, 1976].

References


Davey, W. P. and Hoffman, E. O. (1920). Phys. Rev. 15, 333.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 204.

Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081), p. 8.

Suzuki, T. (1960). Acta Crystallogr. 13, 279.

Swanson, H. E. and Tatge, E. (1953). Nat'l. Bur. Std. U.S. Circ. 539, 1, 43.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 2.7777 | 36 | 1 1 1 | 32.20 |
| 2.4051 | 100 | 2 0 0 | 37.36 |
| 1.7008 | 49 | 2 2 0 | 53.86 |
| 1.4504 | 14 | 3 1 1 | 64.16 |
| 1.3887 | 13 | 2 2 2 | 67.38 |
| 1.2026 | 5 | 4 0 0 | 79.66 |
| 1.1037 | 5 | 3 3 1 | 88.52 |
| 1.0757 | 14 | 4 2 0 | 91.46 |
| .9820 | 11 | 4 2 2 | 103.34 |
| .9259 | 5 | 5 1 1+ | 112.60 |
| .8504 | 4 | 4 4 0 | 129.86 |
| .8132 | 7 | 5 3 1 | 142.62 |
| .8018 | 11 | 4 4 2+ | 147.78 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 2.7775 | 36 | 1 1 1 | 32.20 |
| 2.4054 | 100 | 2 0 0 | 37.35 |
| 1.7009 | 54 | 2 2 0 | 53.86 |
| 1.4505 | 16 | 3 1 1 | 64.15 |
| 1.3888 | 15 | 2 2 2 | 67.38 |
| 1.2027 | 6 | 4 0 0 | 79.65 |
| 1.1037 | 6 | 3 3 1 | 88.52 |
| 1.0757 | 17 | 4 2 0 | 91.46 |
| .9820 | 14 | 4 2 2 | 103.33 |
| .9258 | 5 | 5 1 1 | 112.61 |
| .9258 | 2 | 3 3 3 | 112.61 |
| .8504 | 8 | 4 4 0 | 129.85 |
| .8132 | 16 | 5 3 1 | 142.62 |
| .8018 | 22 | 4 4 2 | 147.77 |
| .8018 | 6 | 6 0 0 | 147.77 |

# Cerium zinc, $CeZn_3$

Structure
Orthorhombic, Amma (63), Z = 4, from powder data. The pattern is nearly identical to that of $PrZn_3$ (space group Pnma) except that for $CeZn_3$, all hkℓ reflections having k+ℓ = 2n+1 were absent, suggesting a change to the A-centered lattice [Bruzzone et al., 1970].

Atom positions
The structure was determined with all atoms in positions 4(c) of Pnma.

Lattice constants
a = 6.644 A
b = 4.627
c = 10.437
[Bruzzone et al., 1970]

CD cell: a = 6.644, b = 10.437, c = 4.627, space group Amam. a/b = 0.6366, c/b = 0.4433.

Volume
320.9 $A^3$

Density
(calculated) 6.961 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Ce^0$, $Zn^0$ [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.512 \times 10^{-3}$

References

Bruzzone, G., Fornasini, M.L. and Merlo, F. (1970). J. Less-Common Metals 22, 253.
Cromer, D. H. and Mann, J. B. (1968). Acta Crystallogr. A24, 361.


Calculated Pattern (Peak heights)

| d(A) | I | hkℓ | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 4.227 | 5 | 0 1 1 | 21.00 |
| 4.103 | 5 | 1 0 2 | 21.64 |
| 3.567 | 10 | 1 1 1 | 24.94 |
| 3.321 | 10 | 2 0 0 | 26.82 |
| 2.611 | 100 | 2 1 1+ | 34.32 |
| 2.564 | 65 | 1 1 3 | 34.96 |
| 2.429 | 15 | 1 0 4 | 36.98 |
| 2.313 | 35 | 0 2 0 | 38.90 |
| 2.132 | 30 | 2 1 3 | 42.36 |
| 2.039 | 15 | 3 0 2 | 44.40 |
| 2.015 | 1 | 1 2 2 | 44.94 |
| 1.962 | 5 | 3 1 1 | 46.24 |
| 1.898 | 5 | 2 2 0 | 47.88 |
| 1.731 | 15 | 0 2 4 | 52.84 |
| 1.689 | 5 | 3 0 4 | 54.28 |
| 1.684 | 5 | 1 0 6 | 54.44 |
| 1.675 | 10 | 1 2 4 | 54.76 |
| 1.661 | 5 | 4 0 0 | 55.26 |
| 1.651 | 10 | 2 1 5 | 55.62 |
| 1.546 | 5 | 4 1 1 | 59.76 |
| 1.530 | 10 | 3 2 2 | 60.48 |
| 1.4432 | 1 | 3 1 5 | 64.52 |
| 1.4258 | 1 | 4 1 3 | 65.40 |
| 1.4193 | 1 | 0 1 7 | 65.74 |
| 1.4012 | 1 | 4 0 4 | 66.70 |
| 1.3872 | 15 | 1 1 7+ | 67.46 |
| 1.3793 | 5 | 1 3 3 | 67.90 |
| 1.3680 | 5 | 3 0 6 | 68.54 |
| 1.3641 | 5 | 3 2 4 | 68.76 |
| 1.3607 | 5 | 1 2 6 | 68.96 |
| 1.3494 | 5 | 4 2 0 | 69.62 |
| 1.2978 | 5 | 2 3 3 | 72.82 |
| 1.2803 | 1 | 1 0 8 | 73.98 |
| 1.2677 | 1 | 5 1 1 | 74.84 |
| 1.2144 | 1 | 2 0 8 | 78.74 |
| 1.1989 | 10 | 5 1 3+ | 79.96 |
| 1.1841 | 1 | 5 0 4 | 81.16 |
| 1.1774 | 5 | 3 2 6 | 81.72 |
| 1.1620 | 1 | 2 3 5 | 83.04 |
| 1.1568 | 1 | 0 4 0 | 83.50 |
| 1.1238 | 1 | 4 3 1+ | 86.54 |
| 1.1203 | 1 | 1 2 8 | 86.88 |
| 1.1073 | 1 | 6 0 0 | 88.16 |
| 1.0752 | 1 | 2 2 8+ | 91.52 |
| 1.0721 | 1 | 0 3 7+ | 91.86 |
| 1.0655 | 1 | 2 1 9 | 92.60 |
| 1.0583 | 5 | 1 3 7+ | 93.42 |
| 1.0443 | 1 | 1 4 4+ | 95.06 |
| 1.0193 | 1 | 6 0 4 | 98.18 |
| 1.0111 | 1 | 3 2 8 | 99.26 |

| Calculated Pattern (Peak heights) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| 1.0061 | 1 | 3 4 2 | 99.92 |
| 1.0020 | 1 | 5 3 1 | 100.48 |
| .9989 | 1 | 6 2 0 | 100.92 |
| .9963 | 1 | 2 0 10 | 101.28 |
| .9699 | 5 | 5 1 7 | 105.16 |
| .9671 | 5 | 5 3 3 | 105.60 |
| .9543 | 1 | 3 4 4 | 107.64 |
| .9514 | 1 | 0 2 10 | 108.12 |
| .9491 | 1 | 4 4 0 | 108.50 |
| .9338 | 1 | 7 0 2+ | 111.16 |
| .9328 | 1 | 6 2 4 | 111.34 |
| .9295 | 1 | 0 1 11 | 111.94 |
| .9146 | 1 | 2 2 10 | 114.76 |
| .8951 | 1 | 2 1 11 | 118.76 |
| .8928 | 1 | 2 3 9 | 119.26 |
| .8921 | 1 | 4 4 4+ | 119.42 |
| .8882 | 1 | 2 5 1 | 120.28 |
| .8863 | 1 | 1 5 3 | 120.72 |
| .8833 | 5 | 3 4 6+ | 121.40 |
| .8741 | 1 | 3 2 10 | 123.58 |
| .8659 | 1 | 7 2 2+ | 125.64 |
| .8636 | 1 | 2 5 3+ | 126.24 |
| .8343 | 5 | 5 3 7 | 134.82 |
| .8332 | 1 | 7 0 6+ | 135.20 |
| .8323 | 1 | 7 2 4 | 135.50 |
| .8255 | 1 | 4 2 10 | 137.84 |
| .8198 | 1 | 2 5 5 | 139.96 |
| .8149 | 1 | 8 1 1 | 141.90 |
| .8111 | 1 | 4 1 11 | 143.50 |
| .8092 | 1 | 3 0 12+ | 144.34 |
| .8081 | 1 | 0 3 11+ | 144.80 |
| .8061 | 1 | 3 4 8+ | 145.72 |
| .7999 | 1 | 6 4 0 | 148.72 |
| .7958 | 1 | 8 1 3 | 150.94 |
| .7889 | 1 | 7 1 7 | 155.06 |
| .7874 | 1 | 7 3 3+ | 156.10 |
| .7854 | 1 | 2 3 11+ | 157.50 |
| .7839 | 1 | 7 2 6 | 158.62 |

| Calculated Pattern (Integrated) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| 4.230 | 5 | 0 1 1 | 20.98 |
| 4.104 | 5 | 1 0 2 | 21.64 |
| 3.568 | 10 | 1 1 1 | 24.93 |
| 3.322 | 10 | 2 0 0 | 26.82 |
| 2.613 | 100 | 2 1 1 | 34.30 |
| 2.609 | 30 | 0 0 4 | 34.34 |
| 2.565 | 80 | 1 1 3 | 34.95 |
| 2.429 | 20 | 1 0 4 | 36.98 |
| 2.313 | 45 | 0 2 0 | 38.90 |
| 2.132 | 35 | 2 1 3 | 42.35 |
| 2.039 | 20 | 3 0 2 | 44.40 |
| 2.015 | 1 | 1 2 2 | 44.94 |
| 1.962 | 5 | 3 1 1 | 46.23 |
| 1.903 | 1 | 0 1 5 | 47.76 |
| 1.898 | 5 | 2 2 0 | 47.88 |
| 1.739 | 1 | 0 0 6 | 52.57 |
| 1.732 | 1 | 3 1 3 | 52.80 |
| 1.731 | 15 | 0 2 4 | 52.85 |
| 1.688 | 5 | 3 0 4 | 54.29 |
| 1.683 | 1 | 1 0 6 | 54.48 |
| 1.675 | 10 | 1 2 4 | 54.75 |
| 1.661 | 5 | 4 0 0 | 55.26 |
| 1.651 | 10 | 2 1 5 | 55.62 |
| 1.546 | 5 | 4 1 1 | 59.77 |
| 1.530 | 15 | 3 2 2 | 60.48 |
| 1.4871 | 1 | 1 3 1 | 62.40 |
| 1.4432 | 1 | 3 1 5 | 64.52 |
| 1.4260 | 1 | 4 1 3 | 65.39 |
| 1.4191 | 5 | 0 1 7 | 65.75 |
| 1.4012 | 1 | 4 0 4 | 66.70 |
| 1.3903 | 1 | 0 2 6 | 67.29 |
| 1.3878 | 15 | 1 1 7 | 67.43 |
| 1.3865 | 10 | 2 3 1 | 67.50 |
| 1.3793 | 10 | 1 3 3 | 67.90 |
| 1.3680 | 5 | 3 0 6 | 68.54 |
| 1.3639 | 5 | 3 2 4 | 68.78 |
| 1.3609 | 1 | 1 2 6 | 68.95 |
| 1.3493 | 5 | 4 2 0 | 69.63 |
| 1.2979 | 5 | 2 3 3 | 72.81 |
| 1.2802 | 1 | 1 0 8 | 73.99 |
| 1.2677 | 1 | 5 1 1 | 74.84 |
| 1.2143 | 1 | 2 0 8 | 78.74 |
| 1.1989 | 10 | 5 1 3 | 79.95 |
| 1.1985 | 1 | 4 2 4 | 79.99 |
| 1.1949 | 1 | 3 1 7 | 80.28 |
| 1.1841 | 1 | 5 0 4 | 81.16 |
| 1.1775 | 10 | 3 2 6 | 81.71 |
| 1.1621 | 5 | 2 3 5 | 83.04 |
| 1.1567 | 5 | 0 4 0 | 83.51 |
| 1.1241 | 1 | 3 0 8 | 86.51 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.1237 | 1 | 4 | 3 | 1 | 86.56 |
| 1.1201 | 1 | 1 | 2 | 8 | 86.90 |
| 1.1073 | 1 | 6 | 0 | 0 | 88.16 |
| 1.0823 | 1 | 3 | 3 | 5 | 90.76 |
| 1.0790 | 1 | 4 | 1 | 7 | 91.11 |
| 1.0752 | 1 | 2 | 2 | 8 | 91.52 |
| 1.0749 | 1 | 4 | 3 | 3 | 91.55 |
| 1.0720 | 1 | 0 | 3 | 7 | 91.87 |
| 1.0712 | 1 | 6 | 1 | 1 | 91.96 |
| 1.0655 | 5 | 2 | 1 | 9 | 92.60 |
| 1.0583 | 5 | 1 | 3 | 7 | 93.42 |
| 1.0575 | 5 | 0 | 4 | 4 | 93.51 |
| 1.0541 | 1 | 5 | 2 | 4 | 93.91 |
| 1.0443 | 1 | 1 | 4 | 4 | 95.05 |
| 1.0437 | 1 | 0 | 0 | 10 | 95.13 |
| 1.0193 | 1 | 6 | 0 | 4 | 98.17 |
| 1.0111 | 1 | 3 | 2 | 8 | 99.26 |
| 1.0061 | 5 | 3 | 4 | 2 | 99.93 |
| 1.0021 | 1 | 5 | 3 | 1 | 100.48 |
| .9988 | 5 | 6 | 2 | 0 | 100.93 |
| .9957 | 1 | 2 | 0 | 10 | 101.36 |
| .9700 | 5 | 5 | 1 | 7 | 105.15 |
| .9670 | 5 | 5 | 3 | 3 | 105.61 |
| .9543 | 1 | 3 | 4 | 4 | 107.65 |
| .9514 | 1 | 0 | 2 | 10 | 108.13 |
| .9492 | 1 | 4 | 4 | 0 | 108.48 |
| .9441 | 1 | 3 | 0 | 10 | 109.35 |
| .9338 | 1 | 7 | 0 | 2 | 111.15 |
| .9328 | 1 | 6 | 2 | 4 | 111.34 |
| .9295 | 1 | 0 | 1 | 11 | 111.94 |
| .9146 | 1 | 2 | 2 | 10 | 114.75 |
| .8951 | 1 | 2 | 1 | 11 | 118.76 |
| .8928 | 1 | 2 | 3 | 9 | 119.26 |
| .8920 | 1 | 4 | 4 | 4 | 119.43 |
| .8920 | 1 | 7 | 0 | 4 | 119.45 |
| .8882 | 5 | 2 | 5 | 1 | 120.28 |
| .8863 | 5 | 1 | 5 | 3 | 120.71 |
| .8837 | 1 | 4 | 0 | 10 | 121.30 |
| .8833 | 5 | 3 | 4 | 6 | 121.40 |
| .8741 | 1 | 3 | 2 | 10 | 123.58 |
| .8730 | 1 | 6 | 1 | 7 | 123.85 |
| .8659 | 1 | 7 | 2 | 2 | 125.63 |
| .8636 | 1 | 2 | 5 | 3 | 126.25 |
| .8583 | 1 | 1 | 4 | 8 | 127.66 |
| .8376 | 1 | 2 | 4 | 8 | 133.76 |
| .8343 | 5 | 5 | 3 | 7 | 134.81 |
| .8332 | 1 | 7 | 0 | 6 | 135.19 |
| .8322 | 1 | 7 | 2 | 4 | 135.51 |
| .8274 | 1 | 5 | 4 | 4 | 137.16 |
| .8255 | 5 | 4 | 2 | 10 | 137.84 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .8198 | 1 | 2 | 5 | 5 | 139.97 |
| .8149 | 5 | 8 | 1 | 1 | 141.90 |
| .8111 | 5 | 4 | 1 | 11 | 143.49 |
| .8081 | 1 | 0 | 3 | 11 | 144.79 |
| .8061 | 1 | 3 | 4 | 8 | 145.70 |
| .8060 | 1 | 4 | 5 | 1 | 145.77 |
| .8022 | 1 | 1 | 3 | 11 | 147.56 |
| .7999 | 5 | 6 | 4 | 0 | 148.73 |
| .7958 | 5 | 8 | 1 | 3 | 150.93 |
| .7907 | 1 | 2 | 2 | 12 | 153.90 |
| .7903 | 1 | 3 | 5 | 5 | 154.17 |
| .7890 | 1 | 7 | 1 | 7 | 155.03 |
| .7874 | 1 | 4 | 5 | 3 | 156.06 |
| .7874 | 1 | 7 | 3 | 3 | 156.10 |
| .7863 | 1 | 0 | 5 | 7 | 156.87 |
| .7855 | 1 | 1 | 1 | 13 | 157.43 |
| .7852 | 1 | 2 | 3 | 11 | 157.61 |
| .7839 | 5 | 7 | 2 | 6 | 158.63 |

# Cerium zinc, $CeZn_5$

Structure
Hexagonal, P6/mmm (191), Z = 1, isostructural with $CaCu_5$, from powder data [Lott and Chiotti, 1966].

Atom positions [ibid.]
1(a) 1 cerium
2(c) 2 zinc
3(g) 3 zinc

Lattice constants
A composition range exists from 70.00 to 71.97 wt.% of zinc, and the constants vary accordingly. For 70 wt.% Zn:

a = 5.4166 Å
c = 4.2649

(published values: a = 5.4163, c = 4.2647 Å [ibid., Table 1])

Volume
108.4 $Å^3$

Density
(calculated) 7.156 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Ce^0$, $Zn^0$ [Cromer and Mann, 1968], corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factors (integrated intensities)
$\gamma = 0.786 \times 10^{-3}$

Additional patterns
1. Green [1973]
2. Lott and Chiotti [1966]

References

Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Green, M. L. (1973). J. Less-Common Metals 32, 391.
Lott, B. G. and Chiotti, P. (1966). Acta Crystallogr. 20, 733.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.69 | 2 | 1 0 0 | 18.92 |
| 4.26 | 4 | 0 0 1 | 20.82 |
| 3.16 | 45 | 1 0 1 | 28.26 |
| 2.707 | 30 | 1 1 0 | 33.06 |
| 2.345 | 35 | 2 0 0 | 38.36 |
| 2.286 | 100 | 1 1 1 | 39.38 |
| 2.132 | 25 | 0 0 2 | 42.36 |
| 2.055 | 12 | 2 0 1 | 44.02 |
| 1.676 | 11 | 1 1 2 | 54.74 |
| 1.637 | 9 | 2 1 1 | 56.14 |
| 1.578 | 16 | 2 0 2 | 58.44 |
| 1.564 | 5 | 3 0 0 | 59.02 |
| 1.468 | 18 | 3 0 1 | 63.30 |
| 1.360 | 3 | 1 0 3 | 68.98 |
| 1.354 | 12 | 2 2 0 | 69.34 |
| 1.261 | 5 | 3 0 2 | 75.32 |
| 1.259 | 10 | 1 1 3 | 75.46 |
| 1.245 | 3 | 3 1 1 | 76.48 |
| 1.216 | 1 | 2 0 3 | 78.64 |
| 1.173 | 2 | 4 0 0 | 82.12 |
| 1.143 | 11 | 2 2 2 | 84.72 |
| 1.131 | 1 | 4 0 1 | 85.88 |
| 1.109 | 2 | 2 1 3 | 87.98 |
| 1.066 | 1 | 0 0 4 | 92.52 |
| 1.052 | 4 | 3 0 3 | 94.16 |
| 1.043 | 2 | 3 2 1 | 95.16 |
| 1.028 | 3 | 4 0 2 | 97.12 |
| 1.024 | 2 | 4 1 0 | 97.62 |
| .995 | 7 | 4 1 1 | 101.40 |
| .993 | 4 | 1 1 4 | 101.76 |
| .971 | 2 | 2 0 4 | 105.04 |
| .960 | 1 | 3 1 3 | 106.76 |
| .923 | 2 | 4 1 2 | 113.18 |
| .887 | 2 | 4 2 0 | 120.66 |
| .883 | 3 | 3 3 1 | 121.42 |
| .881 | 3 | 3 0 4 | 121.94 |
| .858 | 1 | 3 2 3 | 127.72 |
| .839 | 1 | 1 0 5 | 133.24 |
| .838 | 5 | 2 2 4 | 133.72 |
| .831 | 5 | 4 1 3 | 136.04 |
| .827 | 1 | 5 1 1 | 137.48 |
| .819 | 3 | 4 2 2 | 140.44 |
| .814 | 2 | 1 1 5 | 142.46 |
| .789 | 2 | 4 0 4 | 155.06 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 4.69 | 2 | 1 | 0 | 0 | 18.90 |
| 4.26 | 4 | 0 | 0 | 1 | 20.81 |
| 3.16 | 40 | 1 | 0 | 1 | 28.26 |
| 2.708 | 30 | 1 | 1 | 0 | 33.05 |
| 2.345 | 35 | 2 | 0 | 0 | 38.35 |
| 2.286 | 100 | 1 | 1 | 1 | 39.38 |
| 2.132 | 25 | 0 | 0 | 2 | 42.35 |
| 2.055 | 12 | 2 | 0 | 1 | 44.03 |
| 1.675 | 12 | 1 | 1 | 2 | 54.74 |
| 1.637 | 10 | 2 | 1 | 1 | 56.13 |
| 1.578 | 17 | 2 | 0 | 2 | 58.45 |
| 1.564 | 5 | 3 | 0 | 0 | 59.03 |
| 1.468 | 20 | 3 | 0 | 1 | 63.30 |
| 1.361 | 3 | 1 | 0 | 3 | 68.97 |
| 1.354 | 14 | 2 | 2 | 0 | 69.34 |
| 1.261 | 4 | 3 | 0 | 2 | 75.31 |
| 1.259 | 11 | 1 | 1 | 3 | 75.46 |
| 1.244 | 4 | 3 | 1 | 1 | 76.49 |
| 1.216 | 1 | 2 | 0 | 3 | 78.63 |
| 1.173 | 3 | 4 | 0 | 0 | 82.12 |
| 1.143 | 14 | 2 | 2 | 2 | 84.73 |
| 1.131 | 1 | 4 | 0 | 1 | 85.88 |
| 1.109 | 2 | 2 | 1 | 3 | 87.98 |
| 1.066 | 2 | 0 | 0 | 4 | 92.52 |
| 1.052 | 6 | 3 | 0 | 3 | 94.16 |
| 1.043 | 2 | 3 | 2 | 1 | 95.16 |
| 1.028 | 3 | 4 | 0 | 2 | 97.11 |
| 1.024 | 2 | 4 | 1 | 0 | 97.62 |
| .995 | 10 | 4 | 1 | 1 | 101.41 |
| .992 | 2 | 1 | 1 | 4 | 101.87 |
| .971 | 3 | 2 | 0 | 4 | 105.05 |
| .960 | 2 | 3 | 1 | 3 | 106.75 |
| .923 | 3 | 4 | 1 | 2 | 113.17 |
| .916 | 1 | 5 | 0 | 1 | 114.43 |
| .903 | 1 | 3 | 3 | 0 | 117.14 |
| .886 | 3 | 4 | 2 | 0 | 120.67 |
| .883 | 4 | 3 | 3 | 1 | 121.42 |
| .881 | 2 | 3 | 0 | 4 | 121.96 |
| .868 | 1 | 4 | 2 | 1 | 125.12 |
| .858 | 2 | 3 | 2 | 3 | 127.72 |
| .839 | 1 | 1 | 0 | 5 | 133.24 |
| .838 | 9 | 2 | 2 | 4 | 133.71 |
| .831 | 2 | 3 | 3 | 2 | 135.81 |
| .831 | 10 | 4 | 1 | 3 | 136.03 |
| .827 | 2 | 5 | 1 | 1 | 137.48 |
| .819 | 7 | 4 | 2 | 2 | 140.45 |
| .814 | 5 | 1 | 1 | 5 | 142.45 |
| .789 | 5 | 4 | 0 | 4 | 155.06 |
| .783 | 2 | 5 | 0 | 3 | 159.30 |

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with rhombohedral modification of $U_2Zn_{17}$, from powder data and qualitative single crystal analysis [Lott and Chiotti, 1966].

Atom positions
The structures of several analogous compounds have been refined and the atomic parameters are very similar [Johnson et al., 1969]. The parameters for $Ce_2Zn_{17}$ were not available, but the ratios of the cell edges c/a and of the atomic radii $r_{Ce}/r_{Zn}$ are close to the corresponding ratios for $Nb_2Be_{17}$ for which there is refined structure data [Zalkin et al., 1959]. The atomic positions for $Nb_2Be_{17}$ were used here for $Ce_2Zn_{17}$.

| | | | |
|---|---|---|---|
| 6(c) | 6 cerium | 18(f) | 18 zinc(F) |
| 6(c) | 6 zinc(C) | 18(h) | 18 zinc(H) |
| 9(d) | 9 zinc(D) | | |

Lattice constants [Lott and Chiotti]
a = 9.0713(5) Å
c = 13.2852(5)
(published values: a = 9.0708, c = 13.2844)

Volume
946.8 $Å^3$

Density
(calculated) 7.322 $g/cm^3$

Thermal parameters
Isotropic: Zn(C), B = .81; Zn(D), B = 1.32; Zn(F), B = .74; Zn(H), B = 1.04 [Johnson et al., 1969]. For Ce, B = .54, from their values for Pr [ibid.]

Scattering factors
$Ce^0$, $Zn^0$ [Cromer and Mann, 1968], corrected for dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
$\gamma = 0.344 \times 10^{-3}$

References
Cromer, D.T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Cromer, D.T. and Mann, J.B. (1968), Acta. Crystallogr. A24, 321.
Johnson, Q., Smith, G. S. and Wood, D. H. (1969). Acta. Crystallogr. B25, 464.
Lott, B. G. and Chiotti, P. (1966). Acta. Crystallogr. 20, 733.
Zalkin, A., Sands, D.E. and Krikorian, O.H. (1959). Acta. Crystallogr. 12, 713.

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.767 | 5 | 0 2 1 | 23.60 |
| 3.381 | 6 | 2 0 2 | 26.34 |
| 3.169 | 25 | 1 1 3 | 28.14 |
| 3.058 | 9 | 1 0 4 | 29.18 |
| 2.8970 | 2 | 2 1 1 | 30.84 |
| 2.7106 | 7 | 1 2 2 | 33.02 |
| 2.6182 | 40 | 3 0 0 | 34.22 |
| 2.5364 | 20 | 0 2 4 | 35.36 |
| 2.5185 | 4 | 0 1 5 | 35.62 |
| 2.2674 | 65 | 2 2 0 | 39.72 |
| 2.2544 | 100 | 0 3 3+ | 39.96 |
| 2.2140 | 50 | 0 0 6+ | 40.72 |
| 2.2016 | 17 | 2 0 5 | 40.96 |
| 2.1504 | 1 | 1 3 1 | 41.98 |
| 2.0180 | 35 | 2 2 3 | 44.88 |
| 1.9894 | 6 | 1 1 6 | 45.56 |
| 1.9804 | 6 | 1 2 5 | 45.78 |
| 1.9427 | 2 | 4 0 1 | 46.72 |
| 1.8835 | 1 | 0 4 2 | 48.28 |
| 1.8448 | 2 | 1 0 7 | 49.36 |
| 1.8220 | 2 | 1 3 4 | 50.02 |
| 1.7860 | 3 | 3 2 1 | 51.10 |
| 1.7392 | 2 | 2 3 2 | 52.58 |
| 1.7090 | 2 | 0 2 7 | 53.58 |
| 1.6909 | 6 | 3 0 6+ | 54.20 |
| 1.5989 | 11 | 4 1 3+ | 57.60 |
| 1.5844 | 20 | 2 2 6+ | 58.18 |
| 1.5291 | 1 | 5 0 2 | 60.50 |
| 1.5119 | 4 | 3 3 0 | 61.26 |
| 1.4917 | 5 | 2 3 5 | 62.18 |
| 1.4309 | 12 | 3 3 3 | 65.14 |
| 1.4204 | 3 | 0 5 4 | 65.68 |
| 1.4034 | 4 | 1 1 9+ | 66.58 |
| 1.3800 | 2 | 1 5 2 | 67.86 |
| 1.3555 | 4 | 2 4 4+ | 69.26 |
| 1.3521 | 3 | 5 0 5 | 69.46 |
| 1.3093 | 14 | 6 0 0 | 72.08 |
| 1.3064 | 10 | 3 2 7 | 72.26 |
| 1.2987 | 4 | 5 1 4 | 72.76 |
| 1.2959 | 4 | 4 2 5 | 72.94 |
| 1.2859 | 16 | 0 3 9+ | 73.60 |
| 1.2680 | 1 | 0 4 8+ | 74.82 |
| 1.2585 | 1 | 0 2 10+ | 75.48 |
| 1.2484 | 1 | 3 3 6 | 76.20 |
| 1.2462 | 2 | 1 5 5 | 76.36 |
| 1.2371 | 2 | 2 2 9 | 77.02 |
| 1.2102 | 3 | 2 5 3+ | 79.06 |
| 1.1339 | 5 | 4 4 0 | 85.58 |
| 1.1324 | 3 | 5 1 7 | 85.72 |
| 1.1269 | 9 | 0 6 6+ | 86.24 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.1186 | 5 | 4 | 1 | 9+ | 87.04 |
| 1.1071 | 3 | 0 | 0 | 12+ | 88.18 |
| 1.0984 | 1 | 4 | 4 | 3 | 89.06 |
| 1.0752 | 1 | 2 | 6 | 2+ | 91.52 |
| 1.0632 | 1 | 3 | 5 | 4 | 92.86 |
| 1.0562 | 6 | 3 | 3 | 9 | 93.66 |
| 1.0351 | 2 | 6 | 2 | 4 | 96.18 |
| 1.0339 | 1 | 5 | 3 | 5 | 96.32 |
| 1.0197 | 2 | 3 | 0 | 12+ | 98.12 |
| 1.0130 | 3 | 7 | 1 | 3+ | 99.00 |
| 1.0093 | 4 | 4 | 4 | 6 | 99.50 |
| 1.0081 | 2 | 2 | 6 | 5 | 99.66 |
| .9949 | 3 | 2 | 2 | 12 | 101.48 |
| .9898 | 1 | 6 | 3 | 0+ | 102.20 |
| .9660 | 5 | 6 | 3 | 3+ | 105.76 |
| .9574 | 2 | 2 | 5 | 9+ | 107.14 |
| .9449 | 1 | 6 | 2 | 7 | 109.22 |
| .9416 | 1 | 0 | 8 | 4 | 109.78 |
| .9407 | 1 | 4 | 5 | 5 | 109.94 |
| .9220 | 1 | 2 | 7 | 4 | 113.32 |
| .8932 | 1 | 3 | 3 | 12 | 119.18 |
| .8888 | 3 | 3 | 2 | 13+ | 120.14 |
| .8863 | 2 | 8 | 1 | 4 | 120.72 |
| .8821 | 1 | 3 | 4 | 11+ | 121.68 |
| .8689 | 1 | 1 | 8 | 5 | 124.88 |
| .8572 | 4 | 8 | 2 | 0+ | 127.96 |
| .8505 | 3 | 7 | 1 | 9+ | 129.84 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 3.767 | 7 | 0 | 2 | 1 | 23.60 |
| 3.381 | 9 | 2 | 0 | 2 | 26.34 |
| 3.169 | 40 | 1 | 1 | 3 | 28.14 |
| 3.059 | 15 | 1 | 0 | 4 | 29.17 |
| 2.8978 | 3 | 2 | 1 | 1 | 30.83 |
| 2.7108 | 11 | 1 | 2 | 2 | 33.02 |
| 2.6187 | 70 | 3 | 0 | 0 | 34.21 |
| 2.5362 | 40 | 0 | 2 | 4 | 35.36 |
| 2.5170 | 4 | 0 | 1 | 5 | 35.64 |
| 2.2678 | 100 | 2 | 2 | 0 | 39.71 |
| 2.2541 | 85 | 3 | 0 | 3 | 39.97 |
| 2.2541 | 85 | 0 | 3 | 3 | 39.97 |
| 2.2142 | 60 | 0 | 0 | 6 | 40.72 |
| 2.2136 | 30 | 2 | 1 | 4 | 40.73 |
| 2.2008 | 18 | 2 | 0 | 5 | 40.98 |
| 2.1501 | 1 | 1 | 3 | 1 | 41.99 |
| 2.0185 | 60 | 2 | 2 | 3 | 44.87 |
| 1.9898 | 10 | 1 | 1 | 6 | 45.55 |
| 1.9800 | 10 | 1 | 2 | 5 | 45.79 |
| 1.9429 | 4 | 4 | 0 | 1 | 46.72 |
| 1.8834 | 3 | 0 | 4 | 2 | 48.28 |
| 1.8448 | 3 | 1 | 0 | 7 | 49.36 |
| 1.8218 | 3 | 1 | 3 | 4 | 50.03 |
| 1.7859 | 6 | 3 | 2 | 1 | 51.10 |
| 1.7394 | 5 | 2 | 3 | 2 | 52.57 |
| 1.7143 | 1 | 4 | 1 | 0 | 53.40 |
| 1.7089 | 3 | 0 | 2 | 7 | 53.59 |
| 1.6908 | 6 | 3 | 0 | 6 | 54.21 |
| 1.6908 | 5 | 0 | 3 | 6 | 54.21 |
| 1.6848 | 1 | 3 | 1 | 5 | 54.41 |
| 1.5991 | 7 | 2 | 1 | 7 | 57.59 |
| 1.5987 | 8 | 4 | 1 | 3 | 57.61 |
| 1.5987 | 7 | 1 | 4 | 3 | 57.61 |
| 1.5843 | 25 | 2 | 2 | 6 | 58.18 |
| 1.5841 | 12 | 3 | 2 | 4 | 58.19 |
| 1.5603 | 1 | 0 | 5 | 1 | 59.17 |
| 1.5290 | 2 | 5 | 0 | 2 | 60.50 |
| 1.5119 | 7 | 3 | 3 | 0 | 61.26 |
| 1.4915 | 9 | 2 | 3 | 5 | 62.19 |
| 1.4311 | 1 | 1 | 3 | 7 | 65.13 |
| 1.4308 | 25 | 3 | 3 | 3 | 65.15 |
| 1.4203 | 5 | 0 | 5 | 4 | 65.69 |
| 1.4037 | 7 | 1 | 1 | 9 | 66.57 |
| 1.4031 | 2 | 5 | 1 | 1 | 66.60 |
| 1.3802 | 3 | 1 | 5 | 2 | 67.85 |
| 1.3555 | 1 | 4 | 1 | 6 | 69.26 |
| 1.3555 | 1 | 1 | 4 | 6 | 69.26 |
| 1.3554 | 6 | 2 | 4 | 4 | 69.27 |
| 1.3524 | 2 | 5 | 0 | 5 | 69.44 |
| 1.3093 | 25 | 6 | 0 | 0 | 72.08 |

| Calculated Pattern (Integrated) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| 1.3069 | 7 | 3 2 7 | 72.23 |
| 1.2986 | 7 | 5 1 4 | 72.76 |
| 1.2960 | 4 | 4 2 5 | 72.93 |
| 1.2859 | 14 | 3 0 9 | 73.60 |
| 1.2859 | 15 | 0 3 9 | 73.60 |
| 1.2855 | 2 | 4 3 1 | 73.63 |
| 1.2681 | 2 | 0 4 8 | 74.81 |
| 1.2585 | 2 | 0 2 10 | 75.48 |
| 1.2486 | 2 | 3 3 6 | 76.19 |
| 1.2462 | 3 | 1 5 5 | 76.36 |
| 1.2371 | 3 | 2 2 9 | 77.02 |
| 1.2103 | 2 | 0 5 7 | 79.06 |
| 1.2101 | 2 | 5 2 3 | 79.07 |
| 1.2101 | 3 | 2 5 3 | 79.07 |
| 1.1694 | 1 | 2 4 7 | 82.41 |
| 1.1339 | 11 | 4 4 0 | 85.58 |
| 1.1323 | 4 | 5 1 7 | 85.73 |
| 1.1270 | 9 | 6 0 6 | 86.23 |
| 1.1270 | 9 | 0 6 6 | 86.23 |
| 1.1186 | 4 | 4 1 9 | 87.04 |
| 1.1186 | 4 | 1 4 9 | 87.04 |
| 1.1183 | 1 | 3 5 1 | 87.07 |
| 1.1071 | 5 | 0 0 12 | 88.18 |
| 1.1066 | 1 | 5 3 2 | 88.23 |
| 1.1066 | 1 | 0 7 2 | 88.23 |
| 1.0985 | 2 | 4 4 3 | 89.05 |
| 1.0858 | 1 | 6 2 1 | 90.38 |
| 1.0751 | 1 | 2 6 2 | 91.53 |
| 1.0632 | 3 | 3 5 4 | 92.85 |
| 1.0563 | 1 | 3 1 11 | 93.64 |
| 1.0562 | 11 | 3 3 9 | 93.66 |
| 1.0405 | 1 | 7 1 0 | 95.51 |
| 1.0352 | 5 | 6 2 4 | 96.17 |
| 1.0338 | 2 | 5 3 5 | 96.33 |
| 1.0197 | 1 | 0 3 12 | 98.12 |
| 1.0197 | 2 | 3 0 12 | 98.12 |
| 1.0134 | 1 | 1 0 13 | 98.95 |
| 1.0130 | 3 | 7 1 3 | 99.01 |
| 1.0130 | 3 | 1 7 3 | 99.01 |
| 1.0093 | 8 | 4 4 6 | 99.50 |
| 1.0080 | 3 | 2 6 5 | 99.67 |
| 1.0030 | 1 | 5 4 1 | 100.35 |
| .9949 | 6 | 2 2 12 | 101.48 |
| .9900 | 1 | 2 4 10 | 102.17 |
| .9898 | 2 | 6 3 0 | 102.20 |
| .9672 | 1 | 5 1 10 | 105.57 |
| .9663 | 3 | 2 1 13 | 105.72 |
| .9660 | 2 | 3 5 7 | 105.76 |
| .9659 | 4 | 6 3 3 | 105.78 |
| .9659 | 4 | 3 6 3 | 105.78 |

| Calculated Pattern (Integrated) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| .9627 | 2 | 5 4 4 | 106.29 |
| .9575 | 3 | 5 2 9 | 107.13 |
| .9575 | 3 | 2 5 9 | 107.13 |
| .9448 | 2 | 6 2 7 | 109.23 |
| .9417 | 1 | 0 8 4 | 109.77 |
| .9407 | 2 | 4 5 5 | 109.94 |
| .9299 | 1 | 0 7 8 | 111.87 |
| .9252 | 1 | 1 3 13 | 112.72 |
| .9220 | 2 | 2 7 4 | 113.32 |
| .9211 | 1 | 8 0 5 | 113.50 |
| .9173 | 1 | 8 1 1 | 114.23 |
| .9108 | 1 | 1 8 2 | 115.50 |
| .8932 | 2 | 3 3 12 | 119.17 |
| .8890 | 4 | 3 2 13 | 120.11 |
| .8888 | 3 | 5 4 7 | 120.16 |
| .8887 | 1 | 5 5 3 | 120.18 |
| .8861 | 4 | 8 1 4 | 120.75 |
| .8821 | 2 | 3 4 11 | 121.67 |
| .8819 | 1 | 7 3 1 | 121.72 |
| .8689 | 2 | 1 8 5 | 124.87 |
| .8572 | 11 | 8 2 0 | 127.97 |
| .8567 | 2 | 0 5 13 | 128.10 |
| .8565 | 1 | 2 7 7 | 128.15 |
| .8564 | 1 | 9 0 3 | 128.17 |
| .8564 | 2 | 0 9 3 | 128.17 |
| .8505 | 5 | 7 1 9 | 129.84 |
| .8505 | 4 | 1 7 9 | 129.84 |

# Cesium cerium chloride, $Cs_2CeCl_6$

Structure
Hexagonal, $P\bar{3}m1$ (164), Z=1 [Kaatz and Marcovich, 1966].

Atom positions
1(a) 1 cerium
2(d) 2 cesium
6(ℓ) 6 chlorine

Lattice constants [ibid.]
a = 7.476(2) A
c = 6.039(2)

c/a = 0.8078

Volume
292.3 $Å^3$

Density
(calculated) 3.52 $g/cm^3$
[Kaatz and Marcovich, 1966].

Thermal parameters
Isotropic [Kaatz and Marcovich, 1966].

Scattering factors
$Cl^-$ [Dawson, 1960]
$Cs^+$, $Ce^{4+}$ [Thomas and Umeda, 1957]

Scale factors (integrated intensities)
$\gamma = 0.648 \times 10^{-3}$

References
Dawson, B. (1960). Acta Crystallogr. 13, 403.
Kaatz, T. and Marcovich, M. (1966). Acta Crystallogr. 21, 1011.
Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. 6, 293.

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 6.47 | 2 | 100 | 13.68 |
| 6.04 | 4 | 001 | 14.66 |
| 4.41 | 100 | 011 | 20.10 |
| 3.74 | 29 | 110 | 23.80 |
| 3.24 | 2 | 200 | 27.54 |
| 3.18 | 6 | 111 | 28.06 |
| 3.02 | 6 | 002 | 29.56 |
| 2.852 | 6 | 201+ | 31.34 |
| 2.736 | 12 | 102+ | 32.70 |
| 2.267 | 22 | 121 | 39.72 |
| 2.208 | 14 | 202+ | 40.84 |
| 2.158 | 5 | 300 | 41.82 |
| 2.032 | 1 | 301+ | 44.56 |
| 1.922 | 6 | 103 | 47.26 |
| 1.901 | 6 | 212+ | 47.80 |
| 1.869 | 10 | 220 | 48.68 |
| 1.772 | 1 | 113 | 51.52 |
| 1.721 | 8 | 311 | 53.18 |
| 1.710 | 1 | 023 | 53.56 |
| 1.589 | 3 | 222 | 57.98 |
| 1.563 | 1 | 041+ | 59.04 |
| 1.555 | 4 | 213 | 59.40 |
| 1.543 | 3 | 132+ | 59.88 |
| 1.510 | 1 | 004 | 61.36 |
| 1.442 | 4 | 231+ | 64.56 |
| 1.427 | 2 | 042+ | 65.36 |
| 1.413 | 2 | 410 | 66.08 |
| 1.400 | 2 | 114 | 66.78 |
| 1.340 | 2 | 133+ | 70.18 |
| 1.333 | 2 | 322+ | 70.62 |
| 1.266 | 1 | 501 | 74.94 |
| 1.237 | 1 | 304+ | 77.02 |
| 1.195 | 1 | 323+ | 80.26 |
| 1.187 | 1 | 015 | 80.90 |
| 1.174 | 2 | 224 | 81.98 |
| 1.142 | 1 | 151 | 84.84 |
| 1.134 | 1 | 422+ | 85.58 |
| 1.083 | 1 | 125 | 90.68 |
| 1.079 | 1 | 600 | 91.10 |
| 1.032 | 1 | 144+ | 96.62 |
| 1.002 | 1 | 315 | 100.46 |
| 0.9143 | 1 | 531+ | 114.82 |
| .8779 | 1 | 064+ | 122.66 |

| Calculated Pattern (Integrated) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| 6.47 | 2 | 100 | 13.67 |
| 6.04 | 4 | 001 | 14.66 |
| 4.42 | 14 | 101 | 20.09 |
| 4.42 | 100 | 011 | 20.09 |
| 3.74 | 34 | 110 | 23.78 |
| 3.24 | 3 | 200 | 27.53 |
| 3.18 | 8 | 111 | 28.05 |
| 3.02 | 8 | 002 | 29.56 |
| 2.853 | 5 | 201 | 31.33 |
| 2.853 | 2 | 021 | 31.33 |
| 2.737 | 6 | 012 | 32.70 |
| 2.737 | 9 | 102 | 32.70 |
| 2.268 | 3 | 211 | 39.71 |
| 2.268 | 26 | 121 | 39.71 |
| 2.208 | 10 | 202 | 40.83 |
| 2.208 | 9 | 022 | 40.83 |
| 2.158 | 7 | 300 | 41.82 |
| 2.032 | 1 | 301 | 44.55 |
| 1.922 | 7 | 103 | 47.25 |
| 1.922 | 7 | 013 | 47.25 |
| 1.901 | 5 | 212 | 47.80 |
| 1.901 | 3 | 122 | 47.80 |
| 1.869 | 13 | 220 | 48.68 |
| 1.785 | 1 | 221 | 51.12 |
| 1.772 | 1 | 113 | 51.52 |
| 1.721 | 10 | 311 | 53.17 |
| 1.721 | 1 | 131 | 53.17 |
| 1.709 | 1 | 023 | 53.57 |
| 1.599 | 4 | 222 | 57.99 |
| 1.563 | 1 | 041 | 59.04 |
| 1.555 | 6 | 213 | 59.41 |
| 1.543 | 2 | 312 | 59.88 |
| 1.543 | 2 | 132 | 59.88 |
| 1.510 | 2 | 004 | 61.36 |
| 1.442 | 5 | 231 | 64.56 |

| Calculated Pattern (Integrated) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| 1.427 | 2 | 042 | 65.36 |
| 1.427 | 2 | 402 | 65.36 |
| 1.413 | 3 | 410 | 66.08 |
| 1.400 | 2 | 114 | 66.77 |
| 1.370 | 1 | 223 | 68.44 |
| 1.340 | 3 | 133 | 70.18 |
| 1.333 | 1 | 322 | 70.61 |
| 1.333 | 1 | 232 | 70.61 |
| 1.266 | 1 | 501 | 74.95 |
| 1.246 | 1 | 330 | 76.37 |
| 1.237 | 1 | 304 | 77.02 |
| 1.195 | 2 | 323 | 80.26 |
| 1.187 | 1 | 015 | 80.90 |
| 1.174 | 3 | 224 | 81.97 |
| 1.142 | 1 | 151 | 84.85 |
| 1.134 | 1 | 422 | 85.58 |
| 1.134 | 1 | 242 | 85.58 |
| 1.083 | 1 | 125 | 90.67 |
| 1.079 | 1 | 600 | 91.10 |
| 1.048 | 1 | 341 | 94.59 |
| 1.007 | 1 | 513 | 99.82 |
| 1.002 | 1 | 315 | 100.46 |
| 0.9744 | 1 | 611 | 104.47 |
| .9409 | 1 | 433 | 109.90 |
| .9371 | 1 | 235 | 110.57 |
| .9345 | 1 | 440 | 111.03 |
| .9143 | 1 | 531 | 114.82 |
| .8865 | 1 | 163 | 120.68 |
| .8377 | 1 | 155 | 133.72 |
| .8213 | 1 | 451 | 139.42 |
| .8136 | 1 | 217 | 142.43 |
| .7985 | 1 | 345 | 149.43 |
| .7946 | 2 | 444 | 151.59 |
| .7843 | 1 | 721 | 158.33 |

# Chlorpromazine, $C_{17}H_{19}ClN_2S$

Synonym
3-chloro-10-(3'-dimethylamino-n-propyl)-phenothiazine

Stability
The material was unstable in light, air, and x-rays [McDowell, 1969].

Structure
Orthorhombic, Pbca (61), Z = 8. The structure was determined by McDowell [ibid.].

Atom positions
All the atoms were in general positions [ibid.].

Lattice constants [ibid.]
a = 23.50(4) A
b = 15.20(2)
c = 9.23(1)

CD cell: a = 15.20, b = 23.50, c = 9.23, space group Pcab; a/b = 0.6468, c/b = 0.3928

Volume
3297. $Å^3$

Density
(measured) 1.289 g/$cm^3$
(calculated) 1.285 g/$cm^3$

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
$C^0$, $Cl^0$, $N^0$, $S^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.545 \times 10^{-3}$
$I/I_c$ (calculated) = 0.88

References
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), p. 202.
McDowell, J. J. H. (1969). Acta Crystallogr. B25 2175.

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 11.75 | 100 | 2 0 0 | 7.52 |
| 9.28 | 2 | 2 1 0 | 9.52 |
| 7.60 | 13 | 0 2 0 | 11.64 |
| 7.48 | 10 | 1 1 1 | 11.82 |
| 6.54 | 5 | 2 1 1 | 13.52 |
| 6.38 | 1 | 2 2 0 | 13.88 |
| 5.86 | 36 | 0 2 1 | 15.10 |
| 5.69 | 7 | 1 2 1 | 15.56 |
| 5.47 | 7 | 4 1 0 | 16.18 |
| 5.25 | 35 | 2 2 1 | 16.88 |
| 4.69 | 4 | 3 2 1 | 18.92 |
| 4.61 | 41 | 0 0 2 | 19.22 |
| 4.36 | 19 | 1 3 1 | 20.34 |
| 4.30 | 5 | 2 0 2 | 20.66 |
| 4.15 | 75 | 2 3 1 | 21.38 |

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.04 | 6 | 5 1 1 | 22.00 |
| 3.97 | 36 | 3 0 2 | 22.36 |
| 3.89 | 22 | 1 2 2 | 22.86 |
| 3.84 | 9 | 4 3 0+ | 23.16 |
| 3.79 | 4 | 6 1 0+ | 23.44 |
| 3.74 | 4 | 2 2 2 | 23.78 |
| 3.67 | 5 | 5 2 1 | 24.26 |
| 3.63 | 5 | 4 0 2 | 24.52 |
| 3.52 | 16 | 3 2 2+ | 25.26 |
| 3.47 | 8 | 1 4 1 | 25.62 |
| 3.38 | 11 | 1 3 2 | 26.38 |
| 3.27 | 11 | 4 2 2 | 27.22 |
| 3.20 | 5 | 3 4 1 | 27.82 |
| 3.13 | 6 | 3 3 2 | 28.52 |
| 3.09 | 2 | 7 1 1+ | 28.86 |
| 3.02 | 2 | 5 2 2 | 29.54 |
| 2.990 | 2 | 1 1 3 | 29.86 |
| 2.934 | 3 | 8 0 0+ | 30.44 |
| 2.845 | 1 | 2 4 2 | 31.42 |
| 2.813 | 2 | 3 1 3 | 31.78 |
| 2.748 | 3 | 8 1 1+ | 32.56 |
| 2.701 | 4 | 4 5 0+ | 33.14 |
| 2.677 | 6 | 7 3 1+ | 33.44 |
| 2.614 | 3 | 1 3 3 | 34.28 |
| 2.592 | 2 | 4 5 1 | 34.58 |
| 2.556 | 1 | 7 2 2 | 35.08 |
| 2.538 | 1 | 5 1 3+ | 35.34 |
| 2.524 | 1 | 1 5 2 | 35.54 |
| 2.493 | 2 | 3 3 3 | 36.00 |
| 2.477 | 2 | 2 6 0+ | 36.24 |
| 2.400 | 1 | 4 3 3 | 37.44 |
| 2.393 | 1 | 0 4 3 | 37.56 |
| 2.355 | 1 | 8 2 2 | 38.18 |
| 2.342 | 2 | 2 4 3 | 38.40 |
| 2.332 | 3 | 3 6 1 | 38.58 |
| 2.295 | 1 | 5 3 3+ | 39.22 |
| 2.264 | 1 | 2 0 4 | 39.78 |
| 2.255 | 1 | 4 6 1+ | 39.94 |
| 2.244 | 1 | 7 1 3+ | 40.16 |
| 2.234 | 1 | 5 5 2 | 40.34 |
| 2.227 | 1 | 8 3 2 | 40.48 |
| 2.214 | 2 | 4 4 3 | 40.72 |
| 2.209 | 3 | 7 4 2+ | 40.82 |
| 2.177 | 2 | 9 2 2+ | 41.44 |
| 2.130 | 3 | 6 5 2+ | 42.40 |
| 2.127 | 3 | 6 6 0+ | 42.46 |
| 2.105 | 2 | 8 1 3+ | 42.94 |
| 2.084 | 1 | 3 5 3 | 43.38 |
| 2.067 | 4 | 4 2 4+ | 43.76 |
| 2.040 | 1 | 6 4 3 | 44.36 |
| 2.037 | 1 | 4 7 0 | 44.44 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 11.75 | 100 | 2 | 0 | 0 | 7.52 |
| 9.30 | 2 | 2 | 1 | 0 | 9.51 |
| 7.60 | 13 | 0 | 2 | 0 | 11.63 |
| 7.48 | 9 | 1 | 1 | 1 | 11.82 |
| 6.55 | 5 | 2 | 1 | 1 | 13.51 |
| 6.38 | 1 | 2 | 2 | 0 | 13.87 |
| 5.87 | 2 | 4 | 0 | 0 | 15.07 |
| 5.87 | 36 | 0 | 2 | 1 | 15.09 |
| 5.69 | 6 | 1 | 2 | 1 | 15.55 |
| 5.48 | 7 | 4 | 1 | 0 | 16.16 |
| 5.25 | 38 | 2 | 2 | 1 | 16.88 |
| 4.70 | 2 | 3 | 2 | 1 | 18.88 |
| 4.65 | 1 | 4 | 2 | 0 | 19.08 |
| 4.62 | 45 | 0 | 0 | 2 | 19.22 |
| 4.36 | 20 | 1 | 3 | 1 | 20.33 |
| 4.34 | 2 | 1 | 1 | 2 | 20.45 |
| 4.30 | 4 | 2 | 0 | 2 | 20.66 |
| 4.15 | 81 | 2 | 3 | 1 | 21.37 |
| 4.15 | 2 | 4 | 2 | 1 | 21.39 |
| 4.13 | 4 | 2 | 1 | 2 | 21.48 |
| 4.04 | 4 | 5 | 1 | 1 | 22.00 |
| 3.98 | 40 | 3 | 0 | 2 | 22.34 |
| 3.94 | 4 | 0 | 2 | 2 | 22.52 |
| 3.89 | 23 | 1 | 2 | 2 | 22.84 |
| 3.86 | 1 | 3 | 3 | 1 | 23.00 |
| 3.85 | 2 | 3 | 1 | 2 | 23.10 |
| 3.84 | 7 | 4 | 3 | 0 | 23.16 |
| 3.80 | 1 | 0 | 4 | 0 | 23.39 |
| 3.79 | 3 | 6 | 1 | 0 | 23.44 |
| 3.74 | 4 | 2 | 2 | 2 | 23.77 |
| 3.67 | 5 | 5 | 2 | 1 | 24.24 |
| 3.63 | 6 | 4 | 0 | 2 | 24.51 |
| 3.54 | 5 | 4 | 3 | 1 | 25.11 |
| 3.53 | 3 | 4 | 1 | 2 | 25.21 |
| 3.52 | 14 | 3 | 2 | 2 | 25.26 |
| 3.51 | 3 | 0 | 4 | 1 | 25.33 |
| 3.51 | 2 | 6 | 1 | 1 | 25.37 |
| 3.48 | 1 | 6 | 2 | 0 | 25.57 |
| 3.48 | 7 | 1 | 4 | 1 | 25.61 |
| 3.38 | 12 | 1 | 3 | 2 | 26.38 |
| 3.37 | 2 | 2 | 4 | 1 | 26.45 |
| 3.29 | 4 | 5 | 0 | 2 | 27.06 |
| 3.27 | 11 | 4 | 2 | 2 | 27.21 |
| 3.21 | 5 | 3 | 4 | 1 | 27.80 |
| 3.19 | 4 | 4 | 4 | 0 | 27.94 |
| 3.13 | 7 | 3 | 3 | 2 | 28.51 |
| 3.10 | 1 | 6 | 3 | 0 | 28.79 |
| 3.09 | 1 | 7 | 1 | 1 | 28.88 |
| 3.02 | 2 | 5 | 2 | 2 | 29.54 |
| 2.991 | 2 | 1 | 1 | 3 | 29.85 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.950 | 1 | 4 | 3 | 2 | 30.27 |
| 2.937 | 2 | 8 | 0 | 0 | 30.40 |
| 2.934 | 1 | 0 | 4 | 2 | 30.45 |
| 2.930 | 1 | 6 | 1 | 2 | 30.48 |
| 2.846 | 1 | 2 | 4 | 2 | 31.41 |
| 2.814 | 2 | 3 | 1 | 3 | 31.77 |
| 2.753 | 2 | 8 | 1 | 1 | 32.50 |
| 2.747 | 1 | 3 | 4 | 2 | 32.57 |
| 2.709 | 3 | 3 | 5 | 1 | 33.04 |
| 2.700 | 3 | 4 | 5 | 0 | 33.15 |
| 2.683 | 3 | 4 | 1 | 3 | 33.37 |
| 2.678 | 4 | 7 | 3 | 1 | 33.43 |
| 2.673 | 1 | 7 | 1 | 2 | 33.50 |
| 2.625 | 1 | 4 | 4 | 2 | 34.14 |
| 2.613 | 3 | 1 | 3 | 3 | 34.28 |
| 2.591 | 2 | 4 | 5 | 1 | 34.59 |
| 2.557 | 1 | 7 | 2 | 2 | 35.07 |
| 2.538 | 1 | 5 | 1 | 3 | 35.34 |
| 2.524 | 1 | 1 | 5 | 2 | 35.54 |
| 2.493 | 3 | 3 | 3 | 3 | 36.00 |
| 2.476 | 1 | 2 | 6 | 0 | 36.25 |
| 2.400 | 1 | 4 | 3 | 3 | 37.44 |
| 2.391 | 1 | 0 | 4 | 3 | 37.59 |
| 2.356 | 1 | 8 | 2 | 2 | 38.17 |
| 2.343 | 2 | 2 | 4 | 3 | 38.39 |
| 2.332 | 3 | 3 | 6 | 1 | 38.57 |
| 2.295 | 1 | 5 | 3 | 3 | 39.22 |
| 2.264 | 1 | 2 | 0 | 4 | 39.78 |
| 2.256 | 1 | 4 | 6 | 1 | 39.93 |
| 2.243 | 1 | 7 | 1 | 3 | 40.16 |
| 2.234 | 1 | 5 | 5 | 2 | 40.35 |
| 2.226 | 1 | 8 | 3 | 2 | 40.49 |
| 2.215 | 2 | 4 | 4 | 3 | 40.71 |
| 2.209 | 1 | 7 | 4 | 2 | 40.82 |
| 2.177 | 2 | 9 | 2 | 2 | 41.44 |
| 2.137 | 1 | 3 | 6 | 2 | 42.27 |
| 2.130 | 2 | 6 | 5 | 2 | 42.40 |
| 2.127 | 1 | 6 | 6 | 0 | 42.46 |
| 2.104 | 2 | 8 | 1 | 3 | 42.95 |
| 2.084 | 1 | 3 | 5 | 3 | 43.37 |
| 2.073 | 2 | 6 | 6 | 1 | 43.63 |
| 2.070 | 1 | 7 | 3 | 3 | 43.69 |
| 2.067 | 3 | 4 | 2 | 4 | 43.76 |
| 2.062 | 2 | 11 | 1 | 1 | 43.87 |
| 2.041 | 1 | 6 | 4 | 3 | 44.35 |
| 2.037 | 1 | 4 | 7 | 0 | 44.44 |

# Chromium cobalt silicide, $Co_9Cr_{15}Si_6$

Structure
Tetragonal, $P4_2/mnm(136)$, Z = 1, σ-phase, isostructural with σ-(Cr, Fe), from powder data, [Stüwe, 1959]. Much work has been done on the σ-phase structure which has multiple atoms in 5 sites, called A through E [Bergman and Shoemaker, 1954]. The ordering arrangement of the atoms is dependent on a complex combination of electronic and size factors [Spooner, 1968].

Atom positions
The positions used were those for σ-(Cr, Fe) [Spooner and Wilson, 1964], and for σ-(X, Y, Si) [Aronsson and Lundström, 1957]. Site occupancy shared by multiple atoms was assumed to be random and in the following proportions:

| | | |
|---|---|---|
| Site A: | 2(a) | 2.0 cobalt |
| Site B: | 4(f) | 4.0 chromium |
| Site C: | 8(i) | 5.5 chromium and 2.5 cobalt |
| Site D: | 8(i) | 6.0 silicon and 2 cobalt |
| Site E: | 8(j) | 5.5 chromium and 2.5 cobalt |

Lattice constants [Stüwe, 1959]
a = 8.736 Å
c = 4.561

Volume
348.12 $Å^3$

Density
(calculated) 7.054 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Cr^0$, $Si^0$ [Cromer and Mann, 1968].

Scale factor (integrated intensitites)
$\gamma = 0.146 \times 10^{-3}$


References
Aronsson, B. and Lundström, T. (1957). Acta Chem. Scand. 11, 365.
Bergman, G. and Shoemaker, D.P.(1954). Acta Crystallogr. 7, 857.
Cromer, D. T. and Mann, J. B.(1968). Acta Crystallogr. A24, 321.
Spooner, F. J. (1968). Acta Crystallogr. A24, 605.
Spooner, F.J. and Wilson, C.G. (1964). Acta Crystallogr. 17, 1533.
Stüwe, H. P. (1959). Trans. AIME 215, 408.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.904 | 4 | 2 1 0 | 22.76 |
| 3.089 | 3 | 2 2 0 | 28.88 |
| 2.967 | 7 | 2 1 1 | 30.10 |
| 2.455 | 1 | 3 0 1 | 36.58 |
| 2.423 | 2 | 3 2 0 | 37.08 |
| 2.362 | 14 | 3 1 1 | 38.06 |
| 2.281 | 19 | 0 0 2 | 39.48 |
| 2.139 | 5 | 1 1 2 | 42.22 |
| 2.119 | 90 | 4 1 0 | 42.64 |
| 2.059 | 50 | 3 3 0 | 43.94 |
| 2.021 | 50 | 2 0 2 | 44.80 |
| 1.970 | 65 | 2 1 2 | 46.04 |
| 1.922 | 100 | 4 1 1 | 47.26 |
| 1.877 | 35 | 3 3 1 | 48.46 |
| 1.834 | 7 | 2 2 2 | 49.66 |
| 1.758 | 15 | 3 1 2 | 51.96 |
| 1.713 | 1 | 5 1 0 | 53.44 |
| 1.660 | 2 | 3 2 2 | 55.28 |
| 1.632 | 3 | 4 3 1 | 56.34 |
| 1.604 | 1 | 5 1 1 | 57.40 |
| 1.529 | 1 | 5 2 1 | 60.52 |
| 1.387 | 4 | 4 3 2 | 67.48 |
| 1.370 | 2 | 5 1 2+ | 68.44 |
| 1.332 | 1 | 3 1 3 | 70.66 |
| 1.322 | 8 | 5 2 2+ | 71.28 |
| 1.2523 | 15 | 5 3 2 | 75.92 |
| 1.2352 | 19 | 4 1 3+ | 77.16 |
| 1.2272 | 5 | 6 0 2 | 77.76 |
| 1.2232 | 7 | 3 3 3 | 78.06 |
| 1.2154 | 5 | 6 1 2 | 78.66 |
| 1.2036 | 2 | 7 0 1 | 79.58 |
| 1.2001 | 11 | 7 2 0 | 79.86 |
| 1.1924 | 5 | 5 5 1 | 80.48 |
| 1.1815 | 4 | 6 2 2 | 81.38 |
| 1.1708 | 3 | 5 4 2+ | 82.28 |
| 1.1604 | 6 | 7 2 1 | 83.18 |
| 1.1470 | 1 | 4 3 3 | 84.38 |
| 1.1402 | 6 | 0 0 4 | 85.00 |
| 1.0619 | 1 | 7 2 2 | 93.00 |
| 1.0595 | 6 | 8 2 0 | 93.28 |
| 1.0320 | 4 | 8 2 1 | 96.56 |
| 1.0295 | 4 | 6 6 0 | 96.88 |
| 1.0041 | 10 | 4 1 4+ | 100.20 |
| .9976 | 5 | 3 3 4 | 101.10 |
| .9850 | 4 | 8 0 2 | 102.90 |
| .9787 | 7 | 7 4 2 | 103.82 |
| .9609 | 1 | 8 2 2 | 106.58 |
| .9587 | 2 | 5 5 3 | 106.92 |
| .9420 | 3 | 7 2 3 | 109.72 |
| .9277 | 1 | 9 2 1+ | 112.26 |

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| .8886 | 1 | 9 1 2 | 120.20 |
| .8750 | 3 | 7 6 2+ | 123.36 |
| .8692 | 3 | 8 2 3+ | 124.80 |
| .8581 | 1 | 8 5 2+ | 127.72 |
| .8539 | 2 | 9 3 2+ | 128.86 |
| .8525 | 2 | 6 6 3 | 129.26 |
| .8379 | 7 | 4 1 5+ | 133.66 |
| .8340 | 2 | 3 3 5 | 134.92 |
| .8267 | 9 | 7 2 4+ | 137.44 |
| .8231 | 1 | 10 3 1 | 138.74 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.907 | 3 | 2 1 0 | 22.74 |
| 3.089 | 2 | 2 2 0 | 28.88 |
| 2.967 | 6 | 2 1 1 | 30.09 |
| 2.455 | 1 | 3 0 1 | 36.58 |
| 2.423 | 2 | 3 2 0 | 37.07 |
| 2.363 | 13 | 3 1 1 | 38.05 |
| 2.280 | 18 | 0 0 2 | 39.48 |
| 2.139 | 3 | 1 1 2 | 42.21 |
| 2.119 | 85 | 4 1 0 | 42.63 |
| 2.059 | 45 | 3 3 0 | 43.93 |
| 2.022 | 45 | 2 0 2 | 44.80 |
| 1.970 | 65 | 2 1 2 | 46.05 |
| 1.922 | 100 | 4 1 1 | 47.26 |
| 1.877 | 35 | 3 3 1 | 48.46 |
| 1.835 | 7 | 2 2 2 | 49.65 |
| 1.759 | 15 | 3 1 2 | 51.95 |
| 1.713 | 1 | 5 1 0 | 53.43 |
| 1.661 | 2 | 3 2 2 | 55.27 |
| 1.632 | 3 | 4 3 1 | 56.34 |
| 1.604 | 1 | 5 1 1 | 57.40 |
| 1.529 | 1 | 5 2 1 | 60.52 |
| 1.387 | 4 | 4 3 2 | 67.47 |
| 1.370 | 2 | 5 1 2 | 68.43 |
| 1.364 | 1 | 5 4 0 | 68.74 |
| 1.332 | 1 | 3 1 3 | 70.66 |
| 1.322 | 2 | 6 2 1 | 71.27 |
| 1.322 | 7 | 5 2 2 | 71.28 |
| 1.2522 | 17 | 5 3 2 | 75.93 |
| 1.2355 | 5 | 5 5 0 | 77.14 |
| 1.2353 | 17 | 4 1 3 | 77.16 |
| 1.2273 | 5 | 6 0 2 | 77.76 |
| 1.2231 | 7 | 3 3 3 | 78.07 |
| 1.2153 | 6 | 6 1 2 | 78.67 |
| 1.2038 | 1 | 7 0 1 | 79.57 |
| 1.2001 | 12 | 7 2 0 | 79.87 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 1.1925 | 5 | 5 5 1 | 80.47 |
| 1.1815 | 4 | 6 2 2 | 81.38 |
| 1.1709 | 1 | 6 4 1 | 82.27 |
| 1.1709 | 2 | 5 4 2 | 82.28 |
| 1.1606 | 7 | 7 2 1 | 83.17 |
| 1.1469 | 1 | 4 3 3 | 84.38 |
| 1.1402 | 7 | 0 0 4 | 84.99 |
| 1.0699 | 1 | 6 4 2 | 92.10 |
| 1.0620 | 1 | 7 2 2 | 92.99 |
| 1.0595 | 7 | 8 2 0 | 93.28 |
| 1.0320 | 4 | 8 2 1 | 96.56 |
| 1.0296 | 3 | 6 6 0 | 96.86 |
| 1.0043 | 3 | 6 6 1 | 100.17 |
| 1.0041 | 10 | 4 1 4 | 100.20 |
| .9975 | 6 | 3 3 4 | 101.10 |
| .9850 | 4 | 8 0 2 | 102.90 |
| .9788 | 8 | 7 4 2 | 103.82 |
| .9608 | 1 | 8 2 2 | 106.59 |
| .9588 | 3 | 5 5 3 | 106.91 |
| .9420 | 4 | 7 2 3 | 109.72 |
| .8885 | 1 | 9 1 2 | 120.21 |
| .8751 | 2 | 9 2 2 | 123.35 |
| .8751 | 2 | 7 6 2 | 123.35 |
| .8692 | 3 | 8 2 3 | 124.80 |
| .8580 | 1 | 8 5 2 | 127.73 |
| .8539 | 3 | 9 3 2 | 128.87 |
| .8525 | 3 | 6 6 3 | 129.26 |
| .8379 | 5 | 5 5 4 | 133.64 |
| .8379 | 8 | 4 1 5 | 133.67 |
| .8340 | 3 | 3 3 5 | 134.91 |
| .8267 | 5 | 9 4 2 | 137.42 |
| .8266 | 13 | 7 2 4 | 137.46 |
| .8231 | 2 | 10 3 1 | 138.74 |
| .8218 | 1 | 8 4 3 | 139.22 |

# Cobalt copper tin, $CoCu_2Sn$

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with $Cu_2AlMn$, from powder data [Dwight 1967].

Atom positions [ibid.]
4(b) 4 cobalt
8(c) 8 copper
4(a) 4 tin

Lattice constant [ibid.]
a = 5.982 A

Volume
214.1 $A^3$

Density
(calculated) 9.454 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Cu^0$, $Sn^0$ [Cromer and Mann, 1968].

Scale factor (integrated intensities)
$\gamma = 1.42 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Dwight, A.E. (1967). Intermetallic Compounds (Wiley and Sons Inc., New York), Westbrook, J. H. (ed.) p. 174.

Calculated Pattern (Peak heights)

| d(A) | I | hkℓ | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 3.453 | 10 | 1 1 1 | 25.78 |
| 2.990 | 3 | 2 0 0 | 29.86 |
| 2.115 | 100 | 2 2 0 | 42.72 |
| 1.804 | 4 | 3 1 1 | 50.56 |
| 1.496 | 13 | 4 0 0 | 62.00 |
| 1.372 | 1 | 3 3 1 | 68.30 |
| 1.221 | 20 | 4 2 2 | 78.22 |
| 1.151 | 1 | 5 1 1+ | 84.00 |
| 1.057 | 6 | 4 4 0 | 93.52 |
| 1.011 | 1 | 5 3 1 | 99.24 |
| .9458 | 8 | 6 2 0 | 109.06 |
| .8635 | 2 | 4 4 4 | 126.28 |
| .7994 | 13 | 6 4 2 | 149.00 |
| .7788 | 1 | 7 3 1+ | 163.06 |

Calculated Pattern (Integrated)

| d(A) | I | hkℓ | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 3.454 | 9 | 1 1 1 | 25.77 |
| 2.991 | 2 | 2 0 0 | 29.85 |
| 2.115 | 100 | 2 2 0 | 42.72 |
| 1.804 | 4 | 3 1 1 | 50.56 |
| 1.495 | 14 | 4 0 0 | 62.01 |
| 1.372 | 1 | 3 3 1 | 68.29 |
| 1.338 | 1 | 4 2 0 | 70.32 |
| 1.221 | 25 | 4 2 2 | 78.22 |
| 1.151 | 1 | 5 1 1 | 84.00 |
| 1.057 | 7 | 4 4 0 | 93.51 |
| 1.011 | 1 | 5 3 1 | 99.25 |
| .9458 | 11 | 6 2 0 | 109.06 |
| .8634 | 4 | 4 4 4 | 126.29 |
| .7994 | 30 | 6 4 2 | 149.00 |
| .7788 | 1 | 5 5 3 | 163.06 |
| .7788 | 3 | 7 3 1 | 163.06 |

# Cobalt gallium hafnium, $Co_2GaHf$

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with $Cu_2AlMn$, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Atom positions [ibid.]
8(c) 8 cobalt
4(a) 4 gallium
4(b) 4 hafnium

Lattice constant [ibid.]
a = 6.032 A

Volume
219.5 $A^3$

Density
(measured) 11.10 $g/cm^3$ [ibid.]
(calculated) 11.08 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Ga^0$, $Hf^0$ [Cromer and Mann, 1968] corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
$\gamma = 1.287 \times 10^{-3}$

References

Cromer, D.T. and Liberman, D.(1970). J. Chem. Phys. 53, 1891.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Ziebeck, K. R. A. and Webster, P. J. (1974). J. Phys. Chem. Solids 35, 1.


Calculated Pattern (Peak heights)

| d(A) | I | hkℓ | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 3.482 | 20 | 1 1 1 | 25.56 |
| 3.016 | 18 | 2 0 0 | 29.60 |
| 2.132 | 100 | 2 2 0 | 42.36 |
| 1.819 | 9 | 3 1 1 | 50.12 |
| 1.741 | 4 | 2 2 2 | 52.52 |
| 1.508 | 13 | 4 0 0 | 61.44 |
| 1.384 | 3 | 3 3 1 | 67.64 |
| 1.349 | 5 | 4 2 0 | 69.66 |
| 1.231 | 20 | 4 2 2 | 77.46 |
| 1.161 | 2 | 5 1 1+ | 83.14 |
| 1.066 | 6 | 4 4 0 | 92.50 |
| 1.020 | 2 | 5 3 1 | 98.14 |
| 1.005 | 2 | 4 4 2+ | 100.04 |
| .9537 | 8 | 6 2 0 | 107.74 |
| .9198 | 1 | 5 3 3 | 113.74 |
| .9093 | 1 | 6 2 2 | 115.80 |
| .8706 | 2 | 4 4 4 | 124.44 |
| .8446 | 1 | 5 5 1+ | 131.56 |
| .8365 | 1 | 6 4 0 | 134.10 |
| .8061 | 12 | 6 4 2 | 145.74 |
| .7853 | 2 | 7 3 1+ | 157.56 |

Calculated Pattern (Integrated)

| d(A) | I | hkℓ | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 3.483 | 19 | 1 1 1 | 25.56 |
| 3.016 | 17 | 2 0 0 | 29.60 |
| 2.133 | 100 | 2 2 0 | 42.35 |
| 1.819 | 9 | 3 1 1 | 50.12 |
| 1.741 | 5 | 2 2 2 | 52.51 |
| 1.508 | 14 | 4 0 0 | 61.44 |
| 1.384 | 3 | 3 3 1 | 67.65 |
| 1.349 | 6 | 4 2 0 | 69.65 |
| 1.231 | 25 | 4 2 2 | 77.45 |
| 1.161 | 2 | 5 1 1 | 83.14 |
| 1.066 | 7 | 4 4 0 | 92.50 |
| 1.020 | 2 | 5 3 1 | 98.14 |
| 1.005 | 2 | 4 4 2 | 100.03 |
| .9537 | 11 | 6 2 0 | 107.74 |
| .9199 | 1 | 5 3 3 | 113.73 |
| .9094 | 2 | 6 2 2 | 115.79 |
| .8706 | 3 | 4 4 4 | 124.44 |
| .8446 | 1 | 7 1 1 | 131.56 |
| .8446 | 1 | 5 5 1 | 131.56 |
| .8365 | 2 | 6 4 0 | 134.11 |
| .8061 | 30 | 6 4 2 | 145.74 |
| .7853 | 2 | 5 5 3 | 157.57 |
| .7853 | 5 | 7 3 1 | 157.57 |

# Cobalt gallium niobium, $Co_2GaNb$

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with $Cu_2AlMn$, from powder data [Markiv et al., 1965].

Atom positions [ibid.]
8(c) 8 cobalt
4(a) 4 gallium
4(b) 4 niobium

Lattice constant [ibid.]
a = 5.954 A

Volume
211.1 $A^3$

Density
(calculated) 8.826 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Ga^0$, $Nb^0$ [Cromer and Mann, 1968]

Scale factors (integrated intensities)
$\gamma = 1.18 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Markiv, V.Ya., Voroshilov, Yu.V., Kripyakevich, P.I. and Cherkashin, E.E. (1965). Sov. Phys.-Crystallogr. 9, 619.

Calculated Pattern (Peak heights)

| d(A) | I | hkl | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 3.437 | 2 | 1 1 1 | 25.90 |
| 2.976 | 4 | 2 0 0 | 30.00 |
| 2.105 | 100 | 2 2 0 | 42.94 |
| 1.719 | 1 | 2 2 2 | 53.26 |
| 1.488 | 13 | 4 0 0 | 62.34 |
| 1.331 | 1 | 4 2 0 | 70.70 |
| 1.2154 | 20 | 4 2 2 | 78.66 |
| 1.0526 | 6 | 4 4 0 | 94.08 |
| .9414 | 9 | 6 2 0 | 109.82 |
| .8594 | 2 | 4 4 4 | 127.36 |
| .7956 | 14 | 6 4 2 | 151.00 |

Calculated Pattern (Integrated)

| d(A) | I | hkl | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 3.438 | 2 | 1 1 1 | 25.90 |
| 2.977 | 3 | 2 0 0 | 29.99 |
| 2.105 | 100 | 2 2 0 | 42.93 |
| 1.719 | 1 | 2 2 2 | 53.25 |
| 1.488 | 14 | 4 0 0 | 62.33 |
| 1.331 | 1 | 4 2 0 | 70.70 |
| 1.2154 | 25 | 4 2 2 | 78.66 |
| 1.0525 | 7 | 4 4 0 | 94.08 |
| .9414 | 12 | 6 2 0 | 109.82 |
| .8594 | 4 | 4 4 4 | 127.36 |
| .7956 | 35 | 6 4 2 | 151.00 |

# Cobalt germanium, $Co_3Ge_2$

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 1, isostructural with $Ni_2In$ and $Ni_3Sn_2$, from powder data [Lecocq and Michel, 1964].

Atom positions
The structure prototype, $2(Ni_2In)$, has 2 Ni atoms in positions 2(a) and also in 2(d); the indium are in 2(c). Studies on two isostructural compounds, $Ni_3In_2$ and $Co_3Sn_2$, indicated that in their structures the site 2(d) is only partially occupied [Kanematsu, 1962; Rajeswari and Manohar, 1970].

The positions used here for $Co_3Ge_2$ were:
2(a) 2 cobalt
2(d) 1 cobalt
2(c) 2 germanium

Lattice constants [Lecocq and Michel, 1964]
A composition range exists from 36 to 44 atomic percent Ge and the constants vary accordingly. For 40 atomic percent Ge:
a = 3.964 A
c = 4.992

Volume
67.93 $A^3$

Density
(calculated) 7.870 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Ge^0$ [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.418 \times 10^{-3}$

References

Cromer, D. T. and Mann, J. B. (1968) Acta Crystallogr. A24, 321.
Kanematsu, K. (1962). J. Phys. Soc. Jap. 17, 85.
Lecocq, P. and Michel, A. (1964). Bull. Soc. Chim. Fr. 1964, 1911.
Rajeswari, H. and Manohar, H. (1970). Indian J. Pure Appl. Phys. 8, 363.


Calculated Pattern (Peak heights)

| d(A) | I | hkℓ | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 3.432 | 2 | 1 0 0 | 25.94 |
| 2.827 | 35 | 1 0 1 | 31.62 |
| 2.495 | 5 | 0 0 2 | 35.96 |
| 2.019 | 100 | 1 0 2 | 44.86 |
| 1.982 | 100 | 1 1 0 | 45.74 |
| 1.623 | 5 | 2 0 1 | 56.66 |
| 1.552 | 6 | 1 1 2 | 59.50 |
| 1.497 | 4 | 1 0 3 | 61.92 |
| 1.414 | 25 | 2 0 2 | 66.00 |
| 1.256 | 4 | 2 1 1 | 75.68 |
| 1.248 | 5 | 0 0 4 | 76.22 |
| 1.195 | 1 | 2 0 3 | 80.30 |
| 1.151 | 19 | 2 1 2 | 84.00 |
| 1.144 | 10 | 3 0 0 | 84.62 |
| 1.056 | 15 | 1 1 4 | 93.68 |
| 1.040 | 1 | 3 0 2 | 95.56 |
| 1.023 | 2 | 2 1 3 | 97.68 |
| .991 | 6 | 2 2 0 | 102.02 |
| .935 | 1 | 3 1 1 | 110.90 |
| .921 | 1 | 2 2 2 | 113.50 |
| .890 | 8 | 3 1 2 | 119.98 |
| .843 | 8 | 3 0 4 | 131.92 |
| .826 | 1 | 3 1 3 | 137.54 |
| .812 | 3 | 4 0 2 | 143.28 |
| .809 | 4 | 1 0 6 | 144.60 |
| .7913 | 1 | 2 1 5 | 153.56 |
| .7779 | 1 | 3 2 1 | 163.92 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 3.433 | 2 | 1 | 0 | 0 | 25.93 |
| 2.829 | 30 | 1 | 0 | 1 | 31.61 |
| 2.496 | 5 | 0 | 0 | 2 | 35.95 |
| 2.019 | 100 | 1 | 0 | 2 | 44.86 |
| 1.982 | 100 | 1 | 1 | 0 | 45.74 |
| 1.623 | 5 | 2 | 0 | 1 | 56.66 |
| 1.552 | 6 | 1 | 1 | 2 | 59.51 |
| 1.497 | 4 | 1 | 0 | 3 | 61.92 |
| 1.414 | 25 | 2 | 0 | 2 | 66.00 |
| 1.256 | 4 | 2 | 1 | 1 | 75.67 |
| 1.248 | 5 | 0 | 0 | 4 | 76.23 |
| 1.195 | 2 | 2 | 0 | 3 | 80.29 |
| 1.151 | 20 | 2 | 1 | 2 | 83.99 |
| 1.144 | 12 | 3 | 0 | 0 | 84.62 |
| 1.056 | 18 | 1 | 1 | 4 | 93.67 |
| 1.040 | 1 | 3 | 0 | 2 | 95.55 |
| 1.023 | 2 | 2 | 1 | 3 | 97.67 |
| .991 | 7 | 2 | 2 | 0 | 102.03 |
| .959 | 1 | 1 | 0 | 5 | 106.93 |
| .935 | 2 | 3 | 1 | 1 | 110.90 |
| .921 | 1 | 2 | 2 | 2 | 113.51 |
| .890 | 12 | 3 | 1 | 2 | 119.97 |
| .863 | 1 | 2 | 0 | 5 | 126.39 |
| .846 | 1 | 4 | 0 | 1 | 131.21 |
| .843 | 14 | 3 | 0 | 4 | 131.93 |
| .826 | 2 | 3 | 1 | 3 | 137.53 |
| .812 | 8 | 4 | 0 | 2 | 143.29 |
| .809 | 8 | 1 | 0 | 6 | 144.59 |
| .7913 | 3 | 2 | 1 | 5 | 153.56 |
| .7779 | 5 | 3 | 2 | 1 | 163.92 |

# Cobalt germanium hafnium, $Co_{16}Ge_7Hf_6$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Gladyshevs'kii et al., 1962].

Atom positions
The positions are those determined by Bergman and Waugh [1956] for $Cu_{16}Mg_6Si_7$.

| | |
|---|---|
| 32(f) | 32 cobalt(1) |
| 32(f) | 32 cobalt(2) |
| 24(e) | 24 hafnium |
| 4(b) | 4 germanium(1) |
| 24(d) | 24 germanium(2) |

Lattice constant
a = 11.567 Å
(published value, a = 11.566 [Gladyshevs'kii et al., 1962])

Volume
1547.6 $Å^3$

Density
(calculated) 10.824 $g/cm^3$

Thermal parameters
Isotropic: cobalt, B = 1.0; germanium, B = 1.0; hafnium, B = 0.8

Scattering factors
$Co^0$, $Ge^0$, $Hf^0$ [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.370 \times 10^{-3}$

References


Bergman, G. and Waugh, J. L. T. (1956). Acta Crystallogr. 9, 214.

Gladyshevs'kii, E. I., Markiv, V. Ya., and Kuz'ma, Yu.B.(1962). Dopov. Akad. Nauk. Ukr. RSR, No. 4, p. 481.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 204, 212.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 6.672 | 30 | 1 1 1 | 13.26 |
| 5.779 | 6 | 2 0 0 | 15.32 |
| 3.488 | 1 | 3 1 1 | 25.52 |
| 3.339 | 5 | 2 2 2 | 26.68 |
| 2.892 | 9 | 4 0 0 | 30.90 |
| 2.653 | 40 | 3 3 1 | 33.76 |
| 2.586 | 2 | 4 2 0 | 34.66 |
| 2.361 | 40 | 4 2 2 | 38.08 |
| 2.226 | 100 | 3 3 3+ | 40.50 |
| 2.045 | 55 | 4 4 0 | 44.26 |
| 1.955 | 8 | 5 3 1 | 46.40 |
| 1.928 | 30 | 6 0 0+ | 47.10 |
| 1.743 | 7 | 6 2 2 | 52.44 |
| 1.620 | 8 | 5 5 1 | 56.80 |
| 1.604 | 3 | 6 4 0 | 57.40 |
| 1.506 | 4 | 7 3 1+ | 61.54 |
| 1.446 | 5 | 8 0 0 | 64.38 |
| 1.413 | 8 | 7 3 3 | 66.06 |
| 1.403 | 1 | 6 4 4+ | 66.62 |
| 1.363 | 25 | 8 2 2+ | 68.82 |
| 1.336 | 11 | 7 5 1+ | 70.44 |
| 1.327 | 5 | 6 6 2 | 70.98 |
| 1.270 | 4 | 7 5 3+ | 74.70 |
| 1.262 | 11 | 8 4 2 | 75.24 |
| 1.181 | 1 | 8 4 4 | 81.46 |
| 1.163 | 18 | 9 3 3 | 83.00 |
| 1.157 | 2 | 10 0 0 | 83.50 |
| 1.134 | 1 | 8 6 2+ | 85.56 |
| 1.118 | 2 | 7 7 3+ | 87.08 |
| 1.113 | 7 | 6 6 6 | 87.58 |
| 1.079 | 1 | 9 5 3 | 91.14 |
| 1.074 | 1 | 10 4 0 | 91.66 |
| 1.043 | 3 | 11 1 1+ | 95.22 |
| 1.022 | 1 | 8 8 0 | 97.78 |
| 1.011 | 2 | 9 7 1 | 99.32 |
| 1.007 | 5 | 8 8 2 | 99.84 |
| .992 | 1 | 10 6 0 | 101.90 |
| .981 | 1 | 9 7 3 | 103.46 |
| .978 | 5 | 10 6 2 | 103.98 |
| .964 | 4 | 8 8 4+ | 106.10 |
| .954 | 4 | 11 5 1 | 107.68 |
| .938 | 2 | 10 6 4+ | 110.38 |
| .914 | 5 | 12 4 0 | 114.78 |
| .903 | 1 | 8 8 6+ | 117.04 |
| .8924 | 2 | 10 8 2 | 119.34 |
| .8845 | 11 | 11 5 5+ | 121.12 |
| .8823 | 8 | 10 6 6 | 121.64 |
| .8645 | 6 | 13 3 1+ | 126.00 |
| .8622 | 7 | 12 6 0+ | 126.60 |
| .8458 | 2 | 13 3 3 | 131.20 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 6.678 | 40 | 1 | 1 | 1 | 13.25 |
| 5.783 | 8 | 2 | 0 | 0 | 15.31 |
| 4.090 | 1 | 2 | 2 | 0 | 21.71 |
| 3.488 | 2 | 3 | 1 | 1 | 25.52 |
| 3.339 | 8 | 2 | 2 | 2 | 26.68 |
| 2.892 | 15 | 4 | 0 | 0 | 30.90 |
| 2.654 | 65 | 3 | 3 | 1 | 33.75 |
| 2.586 | 2 | 4 | 2 | 0 | 34.65 |
| 2.361 | 70 | 4 | 2 | 2 | 38.08 |
| 2.226 | 80 | 5 | 1 | 1 | 40.49 |
| 2.226 | 95 | 3 | 3 | 3 | 40.49 |
| 2.045 | 100 | 4 | 4 | 0 | 44.26 |
| 1.955 | 14 | 5 | 3 | 1 | 46.40 |
| 1.928 | 40 | 6 | 0 | 0 | 47.10 |
| 1.928 | 17 | 4 | 4 | 2 | 47.10 |
| 1.744 | 14 | 6 | 2 | 2 | 52.43 |
| 1.620 | 15 | 5 | 5 | 1 | 56.79 |
| 1.604 | 6 | 6 | 4 | 0 | 57.40 |
| 1.506 | 6 | 7 | 3 | 1 | 61.53 |
| 1.506 | 2 | 5 | 5 | 3 | 61.53 |
| 1.446 | 9 | 8 | 0 | 0 | 64.38 |
| 1.413 | 16 | 7 | 3 | 3 | 66.06 |
| 1.403 | 1 | 6 | 4 | 4 | 66.62 |
| 1.363 | 20 | 6 | 6 | 0 | 68.81 |
| 1.363 | 25 | 8 | 2 | 2 | 68.81 |
| 1.336 | 13 | 7 | 5 | 1 | 70.44 |
| 1.336 | 9 | 5 | 5 | 5 | 70.44 |
| 1.327 | 9 | 6 | 6 | 2 | 70.98 |
| 1.270 | 2 | 9 | 1 | 1 | 74.70 |
| 1.270 | 7 | 7 | 5 | 3 | 74.70 |
| 1.262 | 20 | 8 | 4 | 2 | 75.23 |
| 1.233 | 1 | 6 | 6 | 4 | 77.32 |
| 1.181 | 3 | 8 | 4 | 4 | 81.46 |
| 1.163 | 35 | 9 | 3 | 3 | 83.00 |
| 1.163 | 2 | 7 | 5 | 5 | 83.00 |
| 1.157 | 2 | 10 | 0 | 0 | 83.51 |
| 1.134 | 1 | 8 | 6 | 2 | 85.55 |
| 1.134 | 1 | 10 | 2 | 0 | 85.55 |
| 1.118 | 3 | 7 | 7 | 3 | 87.08 |
| 1.118 | 1 | 9 | 5 | 1 | 87.08 |
| 1.113 | 13 | 6 | 6 | 6 | 87.59 |
| 1.079 | 2 | 9 | 5 | 3 | 91.15 |
| 1.074 | 2 | 10 | 4 | 0 | 91.66 |
| 1.056 | 1 | 10 | 4 | 2 | 93.69 |
| 1.043 | 6 | 11 | 1 | 1 | 95.22 |
| 1.043 | 1 | 7 | 7 | 5 | 95.22 |
| 1.022 | 2 | 8 | 8 | 0 | 97.78 |
| 1.011 | 4 | 9 | 7 | 1 | 99.32 |
| 1.007 | 11 | 8 | 8 | 2 | 99.83 |
| .992 | 3 | 10 | 6 | 0 | 101.90 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .981 | 3 | 9 | 7 | 3 | 103.47 |
| .978 | 11 | 10 | 6 | 2 | 103.99 |
| .964 | 5 | 8 | 8 | 4 | 106.10 |
| .964 | 4 | 12 | 0 | 0 | 106.10 |
| .954 | 8 | 11 | 5 | 1 | 107.69 |
| .938 | 1 | 12 | 2 | 2 | 110.38 |
| .938 | 3 | 10 | 6 | 4 | 110.38 |
| .929 | 1 | 11 | 5 | 3 | 112.01 |
| .914 | 11 | 12 | 4 | 0 | 114.78 |
| .906 | 1 | 9 | 9 | 1 | 116.47 |
| .903 | 1 | 8 | 8 | 6 | 117.04 |
| .8924 | 5 | 10 | 8 | 2 | 119.35 |
| .8846 | 11 | 11 | 5 | 5 | 121.11 |
| .8846 | 5 | 11 | 7 | 1 | 121.11 |
| .8846 | 11 | 9 | 9 | 3 | 121.11 |
| .8820 | 10 | 10 | 6 | 6 | 121.71 |
| .8646 | 10 | 13 | 3 | 1 | 125.99 |
| .8646 | 2 | 11 | 7 | 3 | 125.99 |
| .8646 | 3 | 9 | 7 | 7 | 125.99 |
| .8622 | 12 | 12 | 6 | 0 | 126.62 |
| .8622 | 3 | 10 | 8 | 4 | 126.62 |
| .8459 | 5 | 13 | 3 | 3 | 131.20 |

# Cobalt germanium niobium, $Co_{16}Ge_7Nb_6$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions of $Co_{16}Nb_6Si_7$ were preferred.

| | |
|---|---|
| 32(f) | 32 cobalt (1) |
| 32(f) | 32 cobalt (2) |
| 4(b) | 4 germanium (1) |
| 24(d) | 24 germanium (2) |
| 24(e) | 24 niobium |

Lattice constant
a = 11.477 Å
(published value, 11.478 Å [Spiegel et al., 1963])

Volume
1511.8 $Å^3$

Density
(calculated) 8.825 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Ge^0$, $Nb^0$ [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.425 \times 10^{-3}$

References


International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), pp. 204, 211.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 5.734 | 4 | 2 0 0 | 15.44 |
| 3.458 | 2 | 3 1 1 | 25.74 |
| 2.868 | 3 | 4 0 0 | 31.16 |
| 2.633 | 19 | 3 3 1 | 34.02 |
| 2.566 | 3 | 4 2 0 | 34.94 |
| 2.342 | 30 | 4 2 2 | 38.40 |
| 2.209 | 80 | 3 3 3+ | 40.82 |
| 2.029 | 100 | 4 4 0 | 44.62 |
| 1.940 | 17 | 5 3 1 | 46.80 |
| 1.913 | 20 | 6 0 0+ | 47.50 |
| 1.815 | 2 | 6 2 0 | 50.24 |
| 1.750 | 3 | 5 3 3 | 52.22 |
| 1.730 | 14 | 6 2 2 | 52.88 |
| 1.607 | 4 | 5 5 1+ | 57.28 |
| 1.494 | 5 | 7 3 1+ | 62.06 |
| 1.434 | 6 | 8 0 0 | 64.96 |
| 1.402 | 5 | 7 3 3 | 66.64 |
| 1.352 | 15 | 8 2 2+ | 69.44 |
| 1.325 | 7 | 5 5 5+ | 71.08 |
| 1.317 | 3 | 6 6 2 | 71.62 |
| 1.283 | 1 | 8 4 0 | 73.78 |
| 1.260 | 7 | 7 5 3+ | 75.40 |
| 1.252 | 7 | 8 4 2 | 75.92 |
| 1.203 | 1 | 9 3 1 | 79.62 |
| 1.171 | 7 | 8 4 4 | 82.24 |
| 1.153 | 14 | 9 3 3 | 83.80 |
| 1.148 | 2 | 8 6 0+ | 84.30 |
| 1.125 | 1 | 10 2 0+ | 86.38 |
| 1.109 | 3 | 7 7 3+ | 87.94 |
| 1.104 | 7 | 6 6 6+ | 88.46 |
| 1.066 | 1 | 10 4 0 | 92.58 |
| 1.035 | 1 | 11 1 1 | 96.20 |
| 1.014 | 3 | 8 8 0 | 98.82 |
| 1.003 | 4 | 9 7 1+ | 100.38 |
| .9990 | 3 | 8 8 2 | 100.90 |
| .9841 | 1 | 8 6 6+ | 103.02 |
| .9700 | 7 | 10 6 2 | 105.14 |
| .9564 | 2 | 12 0 0+ | 107.30 |
| .9467 | 1 | 11 5 1+ | 108.92 |
| .9435 | 1 | 12 2 0 | 109.46 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 5.738 | 3 | 2 | 0 | 0 | 15.43 |
| 3.460 | 2 | 3 | 1 | 1 | 25.72 |
| 2.869 | 3 | 4 | 0 | 0 | 31.15 |
| 2.633 | 17 | 3 | 3 | 1 | 34.02 |
| 2.566 | 2 | 4 | 2 | 0 | 34.93 |
| 2.343 | 30 | 4 | 2 | 2 | 38.39 |
| 2.209 | 35 | 5 | 1 | 1 | 40.82 |
| 2.209 | 40 | 3 | 3 | 3 | 40.82 |
| 2.029 | 100 | 4 | 4 | 0 | 44.63 |
| 1.940 | 17 | 5 | 3 | 1 | 46.79 |
| 1.913 | 17 | 6 | 0 | 0 | 47.49 |
| 1.913 | 4 | 4 | 4 | 2 | 47.49 |
| 1.815 | 2 | 6 | 2 | 0 | 50.24 |
| 1.750 | 3 | 5 | 3 | 3 | 52.22 |
| 1.730 | 14 | 6 | 2 | 2 | 52.87 |
| 1.607 | 1 | 7 | 1 | 1 | 57.28 |
| 1.607 | 3 | 5 | 5 | 1 | 57.28 |
| 1.494 | 4 | 7 | 3 | 1 | 62.07 |
| 1.494 | 1 | 5 | 5 | 3 | 62.07 |
| 1.435 | 7 | 8 | 0 | 0 | 64.95 |
| 1.402 | 6 | 7 | 3 | 3 | 66.65 |
| 1.353 | 9 | 8 | 2 | 2 | 69.43 |
| 1.353 | 8 | 6 | 6 | 0 | 69.43 |
| 1.325 | 4 | 7 | 5 | 1 | 71.08 |
| 1.325 | 4 | 5 | 5 | 5 | 71.08 |
| 1.317 | 3 | 6 | 6 | 2 | 71.62 |
| 1.283 | 1 | 8 | 4 | 0 | 73.78 |
| 1.260 | 1 | 9 | 1 | 1 | 75.39 |
| 1.260 | 7 | 7 | 5 | 3 | 75.39 |
| 1.252 | 7 | 8 | 4 | 2 | 75.92 |
| 1.203 | 1 | 9 | 3 | 1 | 79.62 |
| 1.171 | 8 | 8 | 4 | 4 | 82.24 |
| 1.153 | 15 | 9 | 3 | 3 | 83.80 |
| 1.153 | 1 | 7 | 7 | 1 | 83.80 |
| 1.148 | 1 | 8 | 6 | 0 | 84.31 |
| 1.125 | 1 | 10 | 2 | 0 | 86.39 |
| 1.110 | 1 | 9 | 5 | 1 | 87.94 |
| 1.110 | 2 | 7 | 7 | 3 | 87.94 |
| 1.104 | 1 | 10 | 2 | 2 | 88.45 |
| 1.104 | 6 | 6 | 6 | 6 | 88.45 |
| 1.066 | 1 | 10 | 4 | 0 | 92.58 |
| 1.035 | 2 | 11 | 1 | 1 | 96.21 |
| 1.014 | 4 | 8 | 8 | 0 | 98.81 |
| 1.003 | 3 | 9 | 7 | 1 | 100.38 |
| 1.003 | 1 | 11 | 3 | 1 | 100.38 |
| .9989 | 4 | 8 | 8 | 2 | 100.91 |
| .9700 | 9 | 10 | 6 | 2 | 105.15 |
| .9564 | 1 | 8 | 8 | 4 | 107.30 |
| .9564 | 1 | 12 | 0 | 0 | 107.30 |
| .9466 | 1 | 11 | 5 | 1 | 108.93 |
| .9434 | 1 | 12 | 2 | 0 | 109.47 |

# Cobalt germanium tantalum, $Co_{16}Ge_7Ta_6$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Gladyshevs'kii et al., 1962]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions of $Co_{16}Nb_6Si_7$ were preferred.

| | |
|---|---|
| 32(f) | 32 cobalt(1) |
| 32(f) | 32 cobalt(2) |
| 4(b) | 4 germanium(1) |
| 24(d) | 24 germanium(2) |
| 24(e) | 24 tantalum |

Lattice constant
a = 11.421 A
(published value, 11.420 Å [Gladyshevs'kii et al., 1962]).

Volume
1489.8 $Å^3$

Density
(calculated) 11.310 $g/cm^3$

Thermal parameters
Isotropic: cobalt B = 1.0; germanium B = 1.0; tantalum B = 0.8.

Scattering factors
$Co^0$, $Ge^0$, $Ta^0$ [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.463 \times 10^{-3}$

References


Gladyshevs'kii, E. I., Markiv, V. Ya., and Kuz'ma, Yu. B. (1962). Dopov. Akad. Nauk. Ukr. RSR, No. 4, p. 481.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 204, 212.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I. and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 6.593 | 17 | 1 1 1 | 13.42 |
| 5.705 | 4 | 2 0 0 | 15.52 |
| 4.037 | 3 | 2 2 0 | 22.00 |
| 3.443 | 2 | 3 1 1 | 25.86 |
| 3.295 | 11 | 2 2 2 | 27.04 |
| 2.855 | 14 | 4 0 0 | 31.30 |
| 2.620 | 35 | 3 3 1 | 34.20 |
| 2.553 | 4 | 4 2 0 | 35.12 |
| 2.331 | 40 | 4 2 2 | 38.60 |
| 2.198 | 100 | 3 3 3+ | 41.04 |
| 2.019 | 75 | 4 4 0 | 44.86 |
| 1.930 | 5 | 5 3 1 | 47.04 |
| 1.904 | 25 | 6 0 0+ | 47.74 |
| 1.722 | 3 | 6 2 2 | 53.16 |
| 1.599 | 10 | 5 5 1 | 57.58 |
| 1.584 | 3 | 6 4 0 | 58.20 |
| 1.487 | 9 | 7 3 1+ | 62.40 |
| 1.428 | 5 | 8 0 0 | 65.30 |
| 1.395 | 11 | 7 3 3 | 67.02 |
| 1.385 | 2 | 6 4 4+ | 67.58 |
| 1.346 | 25 | 8 2 2+ | 69.82 |
| 1.319 | 10 | 5 5 5+ | 71.48 |
| 1.310 | 2 | 6 6 2 | 72.02 |
| 1.254 | 5 | 7 5 3 | 75.82 |
| 1.246 | 10 | 8 4 2 | 76.36 |
| 1.166 | 3 | 8 4 4 | 82.72 |
| 1.148 | 15 | 9 3 3+ | 84.30 |
| 1.142 | 2 | 10 0 0 | 84.82 |
| 1.120 | 3 | 8 6 2+ | 86.92 |
| 1.104 | 6 | 7 7 3+ | 88.48 |
| 1.099 | 5 | 6 6 6 | 89.00 |
| 1.060 | 3 | 10 4 0 | 93.18 |
| 1.030 | 2 | 11 1 1 | 96.84 |
| 1.009 | 1 | 8 8 0 | 99.48 |
| .998 | 3 | 9 7 1+ | 101.06 |
| .994 | 6 | 8 8 2 | 101.60 |
| .979 | 2 | 10 6 0 | 103.72 |
| .969 | 1 | 9 7 3 | 105.34 |
| .965 | 6 | 10 6 2 | 105.88 |
| .952 | 3 | 8 8 4+ | 108.06 |
| .942 | 4 | 11 5 1+ | 109.72 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 6.594 | 19 | 1 | 1 | 1 | 13.42 |
| 5.711 | 5 | 2 | 0 | 0 | 15.50 |
| 4.038 | 4 | 2 | 2 | 0 | 21.99 |
| 3.444 | 3 | 3 | 1 | 1 | 25.85 |
| 3.297 | 13 | 2 | 2 | 2 | 27.02 |
| 2.855 | 17 | 4 | 0 | 0 | 31.30 |
| 2.620 | 45 | 3 | 3 | 1 | 34.19 |
| 2.554 | 5 | 4 | 2 | 0 | 35.11 |
| 2.331 | 50 | 4 | 2 | 2 | 38.59 |
| 2.198 | 65 | 5 | 1 | 1 | 41.03 |
| 2.198 | 70 | 3 | 3 | 3 | 41.03 |
| 2.019 | 100 | 4 | 4 | 0 | 44.86 |
| 1.931 | 7 | 5 | 3 | 1 | 47.03 |
| 1.904 | 30 | 6 | 0 | 0 | 47.74 |
| 1.904 | 6 | 4 | 4 | 2 | 47.74 |
| 1.722 | 5 | 6 | 2 | 2 | 53.15 |
| 1.599 | 15 | 5 | 5 | 1 | 57.59 |
| 1.584 | 4 | 6 | 4 | 0 | 58.20 |
| 1.487 | 10 | 7 | 3 | 1 | 62.40 |
| 1.487 | 3 | 5 | 5 | 3 | 62.40 |
| 1.428 | 7 | 8 | 0 | 0 | 65.31 |
| 1.395 | 16 | 7 | 3 | 3 | 67.02 |
| 1.385 | 1 | 8 | 2 | 0 | 67.58 |
| 1.385 | 2 | 6 | 4 | 4 | 67.58 |
| 1.346 | 13 | 6 | 6 | 0 | 69.82 |
| 1.346 | 20 | 8 | 2 | 2 | 69.82 |
| 1.319 | 6 | 7 | 5 | 1 | 71.48 |
| 1.319 | 9 | 5 | 5 | 5 | 71.48 |
| 1.310 | 3 | 6 | 6 | 2 | 72.03 |
| 1.277 | 1 | 8 | 4 | 0 | 74.21 |
| 1.254 | 7 | 7 | 5 | 3 | 75.83 |
| 1.246 | 16 | 8 | 4 | 2 | 76.36 |
| 1.166 | 4 | 8 | 4 | 4 | 82.73 |
| 1.148 | 20 | 9 | 3 | 3 | 84.30 |
| 1.148 | 2 | 7 | 7 | 1 | 84.30 |
| 1.148 | 1 | 7 | 5 | 5 | 84.30 |
| 1.142 | 2 | 10 | 0 | 0 | 84.82 |
| 1.120 | 3 | 8 | 6 | 2 | 86.91 |
| 1.120 | 2 | 10 | 2 | 0 | 86.91 |
| 1.104 | 6 | 7 | 7 | 3 | 88.48 |
| 1.104 | 4 | 9 | 5 | 1 | 88.48 |
| 1.099 | 8 | 6 | 6 | 6 | 89.00 |
| 1.060 | 4 | 10 | 4 | 0 | 93.17 |
| 1.030 | 4 | 11 | 1 | 1 | 96.84 |
| 1.009 | 2 | 8 | 8 | 0 | 99.47 |
| .998 | 1 | 11 | 3 | 1 | 101.06 |
| .998 | 3 | 9 | 7 | 1 | 101.06 |
| .994 | 1 | 10 | 4 | 4 | 101.59 |
| .994 | 9 | 8 | 8 | 2 | 101.59 |
| .979 | 3 | 10 | 6 | 0 | 103.73 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .969 | 2 | 9 | 7 | 3 | 105.34 |
| .965 | 10 | 10 | 6 | 2 | 105.88 |
| .952 | 2 | 12 | 0 | 0 | 108.07 |
| .952 | 3 | 8 | 8 | 4 | 108.07 |
| .942 | 6 | 11 | 5 | 1 | 109.72 |
| .942 | 1 | 7 | 7 | 7 | 109.72 |

# Cobalt hafnium tin, $Co_2HfSn$

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy isostructural with $AlCu_2Mn$, from powder data (x-ray and neutron) [Ziebeck and Webster, 1974].

Atom positions
8(c) 8 cobalt
4(b) 4 hafnium
4(a) 4 tin

Lattice constant
a = 6.218 Å [Table 1, Ziebeck and Webster, 1974].

Volume
240.41 $Å^3$

Density
(calculated) 11.466 $g/cm^3$
(measured) 11.400 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$ $Sn^0$ [Cromer and Mann, 1968]
$Hf^0$ [International Tables, 1974]
All factors were corrected for anomalous dispersion [Cromer and Liberman, 1970].

Scale factor (integrated intensities)
$\gamma = 1.253 \times 10^{-3}$


References
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Cromer, D.T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.
Ziebeck, K.R.A. and Webster, P.J. (1974). J. Phys. Chem. Solids 35, 1.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.590 | 5 | 1 1 1 | 24.78 |
| 3.108 | 25 | 2 0 0 | 28.70 |
| 2.199 | 100 | 2 2 0 | 41.02 |
| 1.875 | 1 | 3 1 1 | 48.52 |
| 1.795 | 5 | 2 2 2 | 50.82 |
| 1.554 | 15 | 4 0 0 | 59.42 |
| 1.390 | 5 | 4 2 0 | 67.28 |
| 1.269 | 20 | 4 2 2 | 74.74 |
| 1.099 | 5 | 4 4 0 | 88.98 |
| 1.036 | 5 | 4 4 2+ | 96.02 |
| .9832 | 10 | 6 2 0 | 103.16 |
| .9374 | 1 | 6 2 2 | 110.52 |
| .8975 | 1 | 4 4 4 | 118.24 |
| .8623 | 1 | 6 4 0 | 126.58 |
| .8309 | 10 | 6 4 2 | 135.96 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.590 | 5 | 1 1 1 | 24.78 |
| 3.109 | 25 | 2 0 0 | 28.69 |
| 2.198 | 100 | 2 2 0 | 41.02 |
| 1.875 | 1 | 3 1 1 | 48.52 |
| 1.795 | 5 | 2 2 2 | 50.83 |
| 1.554 | 15 | 4 0 0 | 59.41 |
| 1.390 | 10 | 4 2 0 | 67.29 |
| 1.269 | 25 | 4 2 2 | 74.73 |
| 1.099 | 5 | 4 4 0 | 88.98 |
| 1.036 | 5 | 4 4 2 | 96.03 |
| 1.036 | 1 | 6 0 0 | 96.03 |
| .9832 | 10 | 6 2 0 | 103.16 |
| .9374 | 5 | 6 2 2 | 110.52 |
| .8975 | 5 | 4 4 4 | 118.25 |
| .8623 | 5 | 6 4 0 | 126.59 |
| .8309 | 25 | 6 4 2 | 135.96 |

# Cobalt holmium, $Co_2Ho$

Structure
Cubic, Fd3m (227), Z = 8, isostructural with $Cu_2Mg$, from powder data [Harris et al., 1965].

Atom positions [ibid.]
8(a) 8 holmium
16(d) 16 cobalt

Lattice constant [ibid.]
a = 7.1734 Å
(published value, 7.1585 kX)

Volume
369.1 $Å^3$

Density
(calculated) 10.177 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Ho^0$ [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 1.07 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Harris, I. R., Mansey, R. C., and Raynor, G. V. (1965). J. Less-Common Metals 9, 270.

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.141 | 20 | 1 1 1 | 21.44 |
| 2.536 | 70 | 2 2 0 | 35.36 |
| 2.162 | 100 | 3 1 1 | 41.74 |
| 2.071 | 14 | 2 2 2 | 43.68 |
| 1.7932 | 1 | 4 0 0 | 50.88 |
| 1.6456 | 4 | 3 3 1 | 55.82 |
| 1.4643 | 20 | 4 2 2 | 63.48 |
| 1.3804 | 25 | 5 1 1+ | 67.84 |
| 1.2680 | 16 | 4 4 0 | 74.82 |
| 1.2126 | 3 | 5 3 1 | 78.88 |
| 1.1342 | 7 | 6 2 0 | 85.56 |
| 1.0940 | 7 | 5 3 3 | 89.52 |
| 1.0815 | 3 | 6 2 2 | 90.84 |
| 1.0045 | 1 | 7 1 1+ | 100.14 |
| .9586 | 9 | 6 4 2 | 106.94 |
| .9339 | 13 | 7 3 1+ | 111.14 |
| .8967 | 3 | 8 0 0 | 118.42 |
| .8454 | 5 | 8 2 2+ | 131.34 |
| .8283 | 8 | 7 5 1+ | 136.86 |
| .8229 | 1 | 6 6 2 | 138.82 |
| .7874 | 2 | 7 5 3+ | 156.08 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.142 | 17 | 1 1 1 | 21.44 |
| 2.536 | 70 | 2 2 0 | 35.36 |
| 2.163 | 100 | 3 1 1 | 41.73 |
| 2.071 | 14 | 2 2 2 | 43.68 |
| 1.7934 | 1 | 4 0 0 | 50.88 |
| 1.6457 | 4 | 3 3 1 | 55.82 |
| 1.4643 | 20 | 4 2 2 | 63.48 |
| 1.3805 | 20 | 5 1 1 | 67.83 |
| 1.3805 | 7 | 3 3 3 | 67.83 |
| 1.2681 | 18 | 4 4 0 | 74.81 |
| 1.2125 | 3 | 5 3 1 | 78.88 |
| 1.1342 | 8 | 6 2 0 | 85.55 |
| 1.0939 | 8 | 5 3 3 | 89.52 |
| 1.0814 | 3 | 6 2 2 | 90.84 |
| 1.0045 | 1 | 7 1 1 | 100.15 |
| 1.0045 | 1 | 5 5 1 | 100.15 |
| .9586 | 11 | 6 4 2 | 106.95 |
| .9339 | 12 | 7 3 1 | 111.14 |
| .9339 | 6 | 5 5 3 | 111.14 |
| .8967 | 4 | 8 0 0 | 118.42 |
| .8764 | 1 | 7 3 3 | 123.04 |
| .8454 | 3 | 6 6 0 | 131.34 |
| .8454 | 6 | 8 2 2 | 131.34 |
| .8283 | 13 | 7 5 1 | 136.86 |
| .8283 | 2 | 5 5 5 | 136.86 |
| .8228 | 3 | 6 6 2 | 138.83 |
| .8020 | 1 | 8 4 0 | 147.67 |
| .7874 | 4 | 7 5 3 | 156.09 |
| .7874 | 2 | 9 1 1 | 156.09 |

# Cobalt iron sulfide, $Co_8FeS_8$

Structure
Cubic, Fm3m (225), Z = 4, π phase, isostructural with $Co_9S_8$, from powder data (neutron and x-ray) [Knop, 1962].

Atom positions [Pearson, 1967]

| | | | |
|---|---|---|---|
| 4(b) | 3.6 cobalt | 32(f) | 3.6 iron |
| 4(b) | 0.4 iron | 24(e) | 8.0 sulfur |
| 32(f) | 28.4 cobalt | 24(e) | 24.0 sulfur |

Lattice constant
a = 9.944(2) Å
(published value, a = 9.943(2) Å, [Knop, 1962])

Volume
983.3 $Å^3$

Density
(calculated) 5.295 $g/cm^3$

Thermal parameters
Isotropic: cobalt, B = 0.5; iron, B = 0.5; sulfur, B = 0.7

Scattering factors
$Co^0$, $Fe^0$, $S^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.319 \times 10^{-3}$

References


International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England). pp. 202, 204.

Knop, D. (1962). Chem. Ind. London, April 21, p. 739.

Pearson, W.B. (1967). Handbook of Lattice Spacings and Structures of Metals and Alloys, v.2, (Pergamon, Press, N.Y.) pp. 197, 788.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 5.734 | 35 | 1 1 1 | 15.44 |
| 4.968 | 6 | 2 0 0 | 17.84 |
| 3.515 | 6 | 2 2 0 | 25.32 |
| 2.998 | 100 | 3 1 1 | 29.78 |
| 2.870 | 25 | 2 2 2 | 31.14 |
| 2.486 | 8 | 4 0 0 | 36.10 |
| 2.281 | 14 | 3 3 1 | 39.48 |
| 2.223 | 3 | 4 2 0 | 40.54 |
| 2.030 | 2 | 4 2 2 | 44.60 |
| 1.913 | 35 | 5 1 1+ | 47.48 |
| 1.758 | 95 | 4 4 0 | 51.98 |
| 1.681 | 5 | 5 3 1 | 54.56 |
| 1.657 | 1 | 4 4 2+ | 55.40 |
| 1.572 | 1 | 6 2 0 | 58.68 |
| 1.516 | 9 | 5 3 3 | 61.06 |
| 1.499 | 5 | 6 2 2 | 61.84 |
| 1.435 | 2 | 4 4 4 | 64.92 |
| 1.392 | 3 | 7 1 1+ | 67.18 |
| 1.329 | 1 | 6 4 2 | 70.86 |
| 1.2947 | 13 | 7 3 1+ | 73.02 |
| 1.2429 | 11 | 8 0 0 | 76.60 |
| 1.2149 | 2 | 7 3 3 | 78.70 |
| 1.1483 | 7 | 7 5 1+ | 84.26 |
| 1.1406 | 2 | 6 6 2 | 84.96 |
| 1.1117 | 1 | 8 4 0 | 87.72 |
| 1.0915 | 2 | 7 5 3 | 89.78 |
| 1.0425 | 5 | 9 3 1 | 95.28 |
| 1.0148 | 20 | 8 4 4 | 98.76 |
| .9994 | 2 | 7 7 1+ | 100.84 |
| .9614 | 6 | 9 5 1+ | 106.50 |
| .9569 | 2 | 10 2 2+ | 107.22 |
| .8966 | 2 | 11 1 1+ | 118.44 |
| .8789 | 8 | 8 8 0 | 122.42 |
| .8688 | 2 | 11 3 1+ | 124.90 |
| .8435 | 3 | 9 7 3+ | 131.92 |
| .8404 | 2 | 10 6 2 | 132.86 |
| .8286 | 1 | 8 8 4+ | 136.74 |
| .8202 | 1 | 11 5 1+ | 139.84 |
| .7987 | 5 | 9 7 5+ | 149.34 |
| .7861 | 17 | 12 4 0 | 156.96 |

Cobalt iron sulfide, $Co_8FeS_8$- (continued)

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 5.741 | 25 | 1 | 1 | 1 | 15.42 |
| 4.972 | 5 | 2 | 0 | 0 | 17.83 |
| 3.516 | 5 | 2 | 2 | 0 | 25.31 |
| 2.998 | 90 | 3 | 1 | 1 | 29.77 |
| 2.871 | 20 | 2 | 2 | 2 | 31.13 |
| 2.486 | 7 | 4 | 0 | 0 | 36.10 |
| 2.281 | 14 | 3 | 3 | 1 | 39.47 |
| 2.224 | 3 | 4 | 2 | 0 | 40.54 |
| 2.030 | 2 | 4 | 2 | 2 | 44.60 |
| 1.914 | 30 | 5 | 1 | 1 | 47.47 |
| 1.914 | 6 | 3 | 3 | 3 | 47.47 |
| 1.758 | 100 | 4 | 4 | 0 | 51.98 |
| 1.681 | 5 | 5 | 3 | 1 | 54.55 |
| 1.657 | 1 | 4 | 4 | 2 | 55.39 |
| 1.572 | 1 | 6 | 2 | 0 | 58.67 |
| 1.516 | 10 | 5 | 3 | 3 | 61.06 |
| 1.499 | 6 | 6 | 2 | 2 | 61.84 |
| 1.435 | 2 | 4 | 4 | 4 | 64.92 |
| 1.392 | 2 | 7 | 1 | 1 | 67.17 |
| 1.329 | 1 | 6 | 4 | 2 | 70.86 |
| 1.2946 | 8 | 7 | 3 | 1 | 73.03 |
| 1.2946 | 6 | 5 | 5 | 3 | 73.03 |
| 1.2430 | 13 | 8 | 0 | 0 | 76.59 |
| 1.2149 | 2 | 7 | 3 | 3 | 78.70 |
| 1.1482 | 7 | 7 | 5 | 1 | 84.27 |
| 1.1482 | 2 | 5 | 5 | 5 | 84.27 |
| 1.1407 | 2 | 6 | 6 | 2 | 84.96 |
| 1.1118 | 2 | 8 | 4 | 0 | 87.71 |
| 1.0915 | 2 | 7 | 5 | 3 | 89.78 |
| 1.0424 | 6 | 9 | 3 | 1 | 95.29 |
| 1.0149 | 30 | 8 | 4 | 4 | 98.75 |
| .9994 | 1 | 7 | 7 | 1 | 100.84 |
| .9613 | 1 | 7 | 7 | 3 | 106.51 |
| .9613 | 6 | 9 | 5 | 1 | 106.51 |
| .9569 | 2 | 10 | 2 | 2 | 107.23 |
| .8966 | 2 | 11 | 1 | 1 | 118.43 |
| .8966 | 2 | 7 | 7 | 5 | 118.43 |
| .8789 | 13 | 8 | 8 | 0 | 122.42 |
| .8688 | 2 | 11 | 3 | 1 | 124.90 |
| .8688 | 1 | 9 | 7 | 1 | 124.90 |
| .8434 | 4 | 9 | 7 | 3 | 131.93 |
| .8434 | 1 | 11 | 3 | 3 | 131.93 |
| .8404 | 3 | 10 | 6 | 2 | 132.86 |
| .8287 | 1 | 8 | 8 | 4 | 136.73 |
| .8202 | 2 | 11 | 5 | 1 | 139.83 |
| .8202 | 1 | 7 | 7 | 7 | 139.83 |
| .7987 | 8 | 9 | 7 | 5 | 149.34 |
| .7987 | 5 | 11 | 5 | 3 | 149.34 |
| .7861 | 50 | 12 | 4 | 0 | 156.96 |

# Cobalt iron vanadium, $Co_{4.35}Fe_{13.47}V_{12.18}$

Structure
Tetragonal, $P4_2/mnm(136)$, Z = 1, σ-phase, isostructural with σ-(Cr,Fe), from powder data [Stüwe, 1959]. Much work has been done on the σ-phase structure which has multiple atoms in 5 sites, called A through E [Bergman and Shoemaker, 1954]. The ordering arrangement of the atoms is dependent on a complex combination of electronic and size factors [Spooner, 1968].

Atom positions
The positions used were those for σ-(Cr,Fe) [Spooner and Wilson, 1964]. Site occupancy shared by multiple atoms was assumed to be random and in the following proportions:

| | | |
|---|---|---|
| Site A: | 2(a) | 0.49 cobalt and 1.51 iron |
| Site B: | 4(f) | 4.0 vanadium |
| Site C: | 8(i) | 7.0 vanadium, 0.24 cobalt, and 0.76 iron |
| Site D: | 8(i) | 1.95 cobalt and 6.05 iron |
| Site E: | 8(j) | 1.66 cobalt, 5.16 iron, and 1.18 vanadium |

Lattice constants [Stüwe, 1959]
a = 8.884 A
c = 4.600

Volume
363.1 $Å^3$

Density
(calculated) 7.45 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Fe^0$, $V^0$ [Cromer and Mann, 1968].

Scale factor (integrated intensities)
$\gamma = 0.136 \times 10^{-3}$


References
Bergman, G. and Shoemaker, D.P.(1954). Acta Crystallogr. 7, 857.
Cromer, D.T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Spooner, F. J. (1968). Acta Crystallogr. A24, 605.
Spooner, F. J. and Wilson, C. G. (1964). Acta Crystallogr. 17, 1533.
Stüwe, H. P. (1959). Trans. AIME 215, 408.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.085 | 8 | 1 0 1 | 21.74 |
| 3.711 | 2 | 1 1 1 | 23.96 |
| 2.398 | 4 | 3 1 1 | 37.48 |
| 2.300 | 20 | 0 0 2 | 39.14 |
| 2.154 | 100 | 4 1 0 | 41.90 |
| 2.094 | 40 | 3 3 0 | 43.16 |
| 2.042 | 35 | 2 0 2 | 44.32 |
| 1.990 | 70 | 2 1 2 | 45.54 |
| 1.951 | 95 | 4 1 1 | 46.50 |
| 1.906 | 50 | 3 3 1 | 47.68 |
| 1.855 | 13 | 2 2 2 | 49.06 |
| 1.780 | 15 | 3 1 2 | 51.30 |
| 1.681 | 4 | 3 2 2 | 54.54 |
| 1.658 | 4 | 4 3 1 | 55.38 |
| 1.630 | 4 | 5 1 1 | 56.42 |
| 1.598 | 1 | 4 0 2 | 57.64 |
| 1.553 | 1 | 5 2 1 | 59.48 |
| 1.406 | 2 | 4 3 2 | 66.44 |
| 1.389 | 2 | 5 1 2 | 67.38 |
| 1.341 | 4 | 5 2 2 | 70.14 |
| 1.2703 | 12 | 5 3 2 | 74.66 |
| 1.2565 | 5 | 5 5 0 | 75.62 |
| 1.2492 | 14 | 4 1 3 | 76.14 |
| 1.2459 | 11 | 6 0 2 | 76.38 |
| 1.2371 | 8 | 3 3 3 | 77.02 |
| 1.2331 | 7 | 6 1 2 | 77.32 |
| 1.2203 | 11 | 7 2 0 | 78.28 |
| 1.2120 | 6 | 5 5 1 | 78.92 |
| 1.1989 | 4 | 6 2 2 | 79.96 |
| 1.1880 | 4 | 5 4 2 | 80.84 |
| 1.1796 | 7 | 7 2 1 | 81.54 |
| 1.1609 | 1 | 4 3 3 | 83.14 |
| 1.1501 | 7 | 0 0 4 | 84.10 |
| 1.0774 | 7 | 8 2 0 | 91.28 |
| 1.0490 | 3 | 8 2 1 | 94.50 |
| 1.0470 | 4 | 6 6 0 | 94.74 |
| 1.0210 | 2 | 6 6 1 | 97.96 |
| 1.0145 | 9 | 4 1 4 | 98.80 |
| 1.0081 | 4 | 3 3 4 | 99.66 |
| 1.0000 | 3 | 8 0 2 | 100.76 |
| .9939 | 7 | 7 4 2 | 101.62 |
| .9757 | 2 | 8 2 2 | 104.28 |
| .9719 | 3 | 5 5 3 | 104.86 |
| .9548 | 3 | 7 2 3 | 107.56 |
| .9431 | 1 | 7 6 1+ | 109.52 |
| .8887 | 2 | 7 6 2+ | 120.16 |
| .8816 | 2 | 8 2 3 | 121.80 |
| .8674 | 2 | 9 3 2 | 125.26 |
| .8647 | 2 | 6 6 3 | 125.96 |
| .8483 | 3 | 5 5 4 | 130.48 |

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| .8461 | 5 | 4 1 5 | 131.12 |
| .8423 | 2 | 3 3 5 | 132.28 |
| .8398 | 3 | 9 4 2 | 133.04 |
| .8369 | 7 | 7 2 4 | 133.96 |
| .8337 | 1 | 8 4 3 | 135.02 |
| .8288 | 2 | 8 6 2+ | 136.70 |
| .8252 | 2 | 10 1 2 | 137.98 |
| .8214 | 2 | 9 6 0 | 139.38 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.085 | 7 | 1 0 1 | 21.74 |
| 3.711 | 2 | 1 1 1 | 23.96 |
| 2.398 | 4 | 3 1 1 | 37.48 |
| 2.300 | 20 | 0 0 2 | 39.13 |
| 2.160 | 2 | 1 1 2 | 41.79 |
| 2.155 | 100 | 4 1 0 | 41.89 |
| 2.094 | 45 | 3 3 0 | 43.17 |
| 2.042 | 35 | 2 0 2 | 44.31 |
| 1.991 | 75 | 2 1 2 | 45.53 |
| 1.987 | 1 | 4 2 0 | 45.63 |
| 1.951 | 100 | 4 1 1 | 46.50 |
| 1.906 | 50 | 3 3 1 | 47.68 |
| 1.856 | 13 | 2 2 2 | 49.05 |
| 1.780 | 15 | 3 1 2 | 51.29 |
| 1.681 | 4 | 3 2 2 | 54.53 |
| 1.658 | 4 | 4 3 1 | 55.38 |
| 1.629 | 4 | 5 1 1 | 56.43 |
| 1.598 | 1 | 4 0 2 | 57.65 |
| 1.553 | 1 | 5 2 1 | 59.47 |
| 1.406 | 2 | 4 3 2 | 66.43 |
| 1.389 | 2 | 5 1 2 | 67.37 |
| 1.344 | 1 | 6 2 1 | 69.97 |
| 1.341 | 4 | 5 2 2 | 70.14 |
| 1.2702 | 14 | 5 3 2 | 74.66 |
| 1.2565 | 5 | 5 5 0 | 75.62 |
| 1.2493 | 16 | 4 1 3 | 76.13 |
| 1.2450 | 8 | 6 0 2 | 76.44 |
| 1.2371 | 9 | 3 3 3 | 77.02 |
| 1.2330 | 6 | 6 1 2 | 77.33 |
| 1.2235 | 1 | 7 0 1 | 78.04 |
| 1.2204 | 12 | 7 2 0 | 78.28 |
| 1.2121 | 7 | 5 5 1 | 78.92 |
| 1.1988 | 4 | 6 2 2 | 79.96 |
| 1.1901 | 1 | 6 4 1 | 80.67 |
| 1.1881 | 4 | 5 4 2 | 80.84 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 1.1796 | 9 | 7 2 1 | 81.54 |
| 1.1609 | 1 | 4 3 3 | 83.14 |
| 1.1511 | 1 | 5 1 3 | 84.01 |
| 1.1500 | 7 | 0 0 4 | 84.11 |
| 1.1477 | 1 | 6 3 2 | 84.31 |
| 1.0780 | 1 | 7 2 2 | 91.21 |
| 1.0774 | 8 | 8 2 0 | 91.28 |
| 1.0490 | 4 | 8 2 1 | 94.50 |
| 1.0470 | 3 | 6 6 0 | 94.73 |
| 1.0209 | 3 | 6 6 1 | 97.96 |
| 1.0146 | 11 | 4 1 4 | 98.80 |
| 1.0080 | 5 | 3 3 4 | 99.67 |
| 1.0001 | 4 | 8 0 2 | 100.75 |
| .9938 | 8 | 7 4 2 | 101.63 |
| .9757 | 2 | 8 2 2 | 104.28 |
| .9719 | 3 | 5 5 3 | 104.86 |
| .9709 | 1 | 8 4 1 | 105.00 |
| .9549 | 4 | 7 2 3 | 107.55 |
| .8888 | 1 | 9 2 2 | 120.15 |
| .8888 | 1 | 7 6 2 | 120.15 |
| .8815 | 3 | 8 2 3 | 121.81 |
| .8674 | 3 | 9 3 2 | 125.27 |
| .8647 | 2 | 6 6 3 | 125.96 |
| .8483 | 4 | 5 5 4 | 130.47 |
| .8461 | 7 | 4 1 5 | 131.12 |
| .8423 | 4 | 3 3 5 | 132.28 |
| .8398 | 5 | 9 4 2 | 133.05 |
| .8369 | 11 | 7 2 4 | 133.96 |
| .8368 | 1 | 10 3 1 | 134.01 |
| .8337 | 1 | 8 4 3 | 135.03 |
| .8288 | 4 | 8 6 2 | 136.70 |
| .8288 | 1 | 10 0 2 | 136.70 |
| .8252 | 4 | 10 1 2 | 137.97 |
| .8214 | 4 | 9 6 0 | 139.38 |

# Cobalt manganese silicide, $Co_2MnSi$

Structure
Cubic, Fm3m (225), Z = 4, a Heusler alloy, isostructural with $AlCu_2Mn$, from powder data [Gladyshevs'kii et al., 1962].

Atom positions
8(c) 8 cobalt
4(b) 4 manganese
4(a) 4 silicon

Lattice constant
a = 5.670 Å [Gladyshevs'kii et al., 1962]

Volume
182.3 $Å^3$

Density
(calculated) 7.320 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Mn^0$, $Si^0$ [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.599 \times 10^{-3}$

References
Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Gladyshevs'kii, E.I., Kripyakevich, P.I., Teslyuk, M.Yu., Zarechnyuk, O. S. and Kuz'ma, Yu.B. (1962). Sov. Phys. Crystallogr. 6, 207.

Calculated Pattern (Peak Heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.274 | 5 | 1 1 1 | 27.22 |
| 2.834 | 5 | 2 0 0 | 31.54 |
| 2.004 | 100 | 2 2 0 | 45.20 |
| 1.710 | 1 | 3 1 1 | 53.56 |
| 1.636 | 1 | 2 2 2 | 56.16 |
| 1.417 | 10 | 4 0 0 | 65.84 |
| 1.268 | 1 | 4 2 0 | 74.82 |
| 1.157 | 20 | 4 2 2 | 83.44 |
| 1.002 | 5 | 4 4 0 | 100.44 |
| .8965 | 10 | 6 2 0 | 118.46 |
| .8184 | 1 | 4 4 4 | 140.52 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.274 | 5 | 1 1 1 | 27.22 |
| 2.835 | 5 | 2 0 0 | 31.53 |
| 2.005 | 100 | 2 2 0 | 45.20 |
| 1.710 | 1 | 3 1 1 | 53.56 |
| 1.637 | 1 | 2 2 2 | 56.15 |
| 1.418 | 15 | 4 0 0 | 65.83 |
| 1.268 | 1 | 4 2 0 | 74.83 |
| 1.157 | 20 | 4 2 2 | 83.45 |
| 1.002 | 5 | 4 4 0 | 100.44 |
| .8965 | 10 | 6 2 0 | 118.46 |
| .8184 | 5 | 4 4 4 | 140.52 |

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with $Ni_3Sn$. The structure was determined by Alte da Veiga [1965].

Atom positions
6(h) 6 cobalt
2(c) 2 molybdenum

Lattice constants
a = 5.125 A
c = 4.113
(published values: a = 5.1245 [±.0015] and c = 4.1125 [±.0020]) [Alte da Veiga, 1965].

c/a = 0.8025

Volume
93.56 $Å^3$

Density
(calculated) 9.682 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^{2+}$, $Mo^{+}$ [Forsyth and Wells, 1959]; corrected for dispersion using Δf' values from Dauben and Templeton [1955].

Scale factors (integrated intensities)
$\gamma = 0.468 \times 10^{-3}$
$I/I_c$ (calculated) = 7.6

References
Alte da Veiga, L.H. (1965). Acta Crystallogr. 18, 857.
Dauben, C. H., and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
Forsyth, J.B. and Wells, M. (1959). Acta Crystallogr. 12, 412.

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.436 | 3 | 1 0 0 | 20.00 |
| 3.016 | 12 | 1 0 1 | 29.60 |
| 2.562 | 4 | 1 1 0 | 35.00 |
| 2.219 | 27 | 2 0 0 | 40.62 |
| 2.056 | 27 | 0 0 2 | 44.00 |
| 1.953 | 100 | 2 0 1 | 46.46 |
| 1.677 | 1 | 2 1 0 | 54.68 |
| 1.604 | 2 | 1 1 2 | 57.40 |
| 1.553 | 2 | 2 1 1 | 59.46 |
| 1.508 | 11 | 2 0 2 | 61.42 |
| 1.310 | 1 | 1 0 3 | 72.04 |
| 1.300 | 1 | 2 1 2 | 72.68 |
| 1.281 | 11 | 2 2 0 | 73.92 |
| 1.179 | 1 | 3 1 1 | 81.56 |
| 1.166 | 11 | 2 0 3 | 82.66 |
| 1.109 | 1 | 4 0 0 | 87.94 |
| 1.087 | 11 | 2 2 2 | 90.20 |
| 1.071 | 7 | 4 0 1 | 91.96 |
| 1.028 | 1 | 0 0 4 | 97.04 |
| .988 | 1 | 3 2 1 | 102.40 |
| .976 | 2 | 4 0 2 | 104.16 |
| .933 | 2 | 2 0 4 | 111.30 |
| .876 | 1 | 4 1 2+ | 123.06 |
| .863 | 4 | 4 0 3 | 126.52 |
| .8388 | 1 | 4 2 0 | 133.38 |
| .8218 | 7 | 4 2 1 | 139.20 |
| .8174 | 1 | 3 2 3 | 140.90 |
| .8019 | 5 | 2 2 4 | 147.70 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.438 | 3 | 1 0 0 | 19.99 |
| 3.017 | 11 | 1 0 1 | 29.59 |
| 2.563 | 4 | 1 1 0 | 34.99 |
| 2.219 | 26 | 2 0 0 | 40.62 |
| 2.056 | 27 | 0 0 2 | 44.00 |
| 1.953 | 100 | 2 0 1 | 46.46 |
| 1.678 | 1 | 2 1 0 | 54.67 |
| 1.604 | 2 | 1 1 2 | 57.41 |
| 1.553 | 2 | 2 1 1 | 59.46 |
| 1.508 | 12 | 2 0 2 | 61.42 |
| 1.310 | 1 | 1 0 3 | 72.04 |
| 1.300 | 1 | 2 1 2 | 72.68 |
| 1.281 | 12 | 2 2 0 | 73.91 |
| 1.201 | 1 | 3 0 2 | 79.79 |
| 1.179 | 1 | 3 1 1 | 81.56 |
| 1.166 | 12 | 2 0 3 | 82.66 |
| 1.110 | 2 | 4 0 0 | 87.93 |
| 1.087 | 12 | 2 2 2 | 90.20 |
| 1.071 | 9 | 4 0 1 | 91.95 |
| 1.028 | 2 | 0 0 4 | 97.03 |
| .988 | 1 | 3 2 1 | 102.40 |
| .977 | 2 | 4 0 2 | 104.15 |
| .933 | 2 | 2 0 4 | 111.31 |
| .916 | 1 | 3 1 3 | 114.49 |
| .876 | 1 | 4 1 2 | 123.07 |
| .863 | 6 | 4 0 3 | 126.53 |
| .8388 | 2 | 4 2 0 | 133.38 |
| .8219 | 15 | 4 2 1 | 139.19 |
| .8174 | 1 | 3 2 3 | 140.89 |
| .8019 | 12 | 2 2 4 | 147.71 |

Structure
Orthorhombic, Pnma (62), Z = 4, isostructural with MnP. The structure was refined by Rundqvist [1962].

Atom positions
All atoms were located in positions 4(c).

Lattice constants
a = 5.077 A
b = 3.281
c = 5.587
[Rundqvist, 1962].

CD cell: a = 5.077, b = 5.587, c = 3.281, space group Pnam, a/b = 0.9087, c/b = 0.5873.

Volume
93.07 $Å^3$

Density
(calculated) 6.417 $g/cm^3$

Thermal parameters
Isotropic: overall B = 0.29

Scattering factors
$Co^0$, $P^0$ [International Tables, 1962]. The cobalt factors were corrected for dispersion [Dauben and Templeton, 1955].

Scale factors (integrated intensities)
$\gamma = 0.158 \times 10^{-3}$
$I/I_c$ (calculated) = 2.28

References
Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 841.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 210.
Rundqvist, S. (1962). Acta Chem. Scand. 16, 287.

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 3.757 | 7 | 1 0 1 | 23.66 |
| 2.829 | 68 | 0 1 1 | 31.60 |
| 2.793 | 20 | 0 0 2 | 32.02 |
| 2.538 | 18 | 2 0 0 | 35.34 |
| 2.472 | 41 | 1 1 1 | 36.32 |
| 2.447 | 20 | 1 0 2 | 36.70 |
| 2.311 | 2 | 2 0 1 | 38.94 |
| 2.008 | 7 | 2 1 0 | 45.12 |
| 1.962 | 51 | 1 1 2 | 46.24 |
| 1.889 | 100 | 2 1 1 | 48.12 |
| 1.879 | 46 | 2 0 2 | 48.40 |
| 1.748 | 19 | 1 0 3 | 52.28 |
| 1.640 | 26 | 0 2 0 | 56.02 |
| 1.631 | 4 | 2 1 2 | 56.38 |
| 1.620 | 38 | 0 1 3+ | 56.80 |
| 1.502 | 3 | 2 0 3 | 61.72 |
| 1.452 | 1 | 3 1 1 | 64.06 |
| 1.415 | 3 | 0 2 2 | 65.98 |
| 1.378 | 3 | 2 2 0 | 67.98 |
| 1.363 | 5 | 1 2 2 | 68.84 |
| 1.347 | 2 | 1 0 4 | 69.78 |
| 1.338 | 1 | 2 2 1 | 70.32 |
| 1.269 | 4 | 4 0 0 | 74.74 |
| 1.253 | 5 | 3 0 3 | 75.90 |
| 1.246 | 9 | 1 1 4 | 76.38 |
| 1.236 | 14 | 2 2 2 | 77.12 |
| 1.224 | 2 | 2 0 4 | 78.02 |
| 1.196 | 8 | 1 2 3 | 80.16 |
| 1.184 | 2 | 4 1 0 | 81.20 |
| 1.158 | 9 | 4 1 1 | 83.40 |
| 1.155 | 8 | 4 0 2 | 83.64 |
| 1.153 | 9 | 3 2 1 | 83.88 |
| 1.108 | 2 | 2 2 3 | 88.12 |
| 1.091 | 6 | 1 0 5 | 89.80 |
| 1.073 | 2 | 0 3 1 | 91.72 |
| 1.050 | 2 | 1 3 1 | 94.38 |
| 1.049 | 2 | 4 0 3 | 94.52 |
| 1.041 | 2 | 1 2 4 | 95.46 |
| 1.036 | 2 | 1 1 5 | 96.12 |
| 1.023 | 15 | 3 1 4 | 97.64 |
| 1.004 | 4 | 4 2 0 | 100.22 |
| .999 | 6 | 1 3 2+ | 100.96 |
| .996 | 6 | 3 2 3 | 101.38 |
| .989 | 9 | 2 3 1 | 102.38 |
| .981 | 2 | 2 2 4 | 103.50 |
| .945 | 4 | 4 2 2 | 109.24 |
| .943 | 5 | 0 3 3 | 109.54 |
| .932 | 1 | 3 0 5 | 111.40 |
| .916 | 7 | 5 1 2 | 114.42 |
| .909 | 8 | 1 2 5 | 115.94 |
| .892 | 2 | 5 0 3 | 119.54 |
| .884 | 3 | 4 2 3 | 121.32 |
| .882 | 5 | 1 1 6 | 121.66 |
| .874 | 2 | 2 0 6 | 123.56 |
| .8490 | 3 | 1 3 4 | 130.28 |
| .8462 | 3 | 6 0 0 | 131.10 |
| .8447 | 1 | 2 1 6 | 131.54 |
| .8285 | 1 | 4 3 0 | 136.78 |
| .8202 | 4 | 0 4 0 | 139.82 |
| .8195 | 5 | 4 3 1+ | 140.08 |
| .8107 | 4 | 6 1 1+ | 143.68 |
| .8098 | 2 | 6 0 2+ | 144.04 |
| .7967 | 1 | 5 1 4 | 150.40 |
| .7943 | 1 | 4 3 2 | 151.74 |
| .7917 | 4 | 3 1 6 | 153.28 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 3.757 | 6 | 1 | 0 | 1 | 23.66 |
| 2.829 | 62 | 0 | 1 | 1 | 31.60 |
| 2.794 | 17 | 0 | 0 | 2 | 32.01 |
| 2.539 | 17 | 2 | 0 | 0 | 35.33 |
| 2.471 | 38 | 1 | 1 | 1 | 36.32 |
| 2.447 | 18 | 1 | 0 | 2 | 36.69 |
| 2.311 | 2 | 2 | 0 | 1 | 38.94 |
| 2.008 | 7 | 2 | 1 | 0 | 45.12 |
| 1.962 | 52 | 1 | 1 | 2 | 46.24 |
| 1.889 | 100 | 2 | 1 | 1 | 48.12 |
| 1.879 | 38 | 2 | 0 | 2 | 48.41 |
| 1.748 | 20 | 1 | 0 | 3 | 52.28 |
| 1.640 | 28 | 0 | 2 | 0 | 56.01 |
| 1.630 | 2 | 2 | 1 | 2 | 56.39 |
| 1.620 | 12 | 3 | 0 | 1 | 56.80 |
| 1.620 | 28 | 0 | 1 | 3 | 56.80 |
| 1.502 | 2 | 2 | 0 | 3 | 61.73 |
| 1.452 | 2 | 3 | 1 | 1 | 64.06 |
| 1.415 | 3 | 0 | 2 | 2 | 65.99 |
| 1.378 | 4 | 2 | 2 | 0 | 67.98 |
| 1.363 | 5 | 1 | 2 | 2 | 68.84 |
| 1.347 | 3 | 1 | 0 | 4 | 69.78 |
| 1.338 | 1 | 2 | 2 | 1 | 70.31 |
| 1.269 | 5 | 4 | 0 | 0 | 74.73 |
| 1.252 | 5 | 3 | 0 | 3 | 75.91 |
| 1.246 | 9 | 1 | 1 | 4 | 76.38 |
| 1.238 | 1 | 4 | 0 | 1 | 76.98 |
| 1.236 | 16 | 2 | 2 | 2 | 77.13 |
| 1.224 | 2 | 2 | 0 | 4 | 78.02 |
| 1.196 | 9 | 1 | 2 | 3 | 80.16 |
| 1.184 | 2 | 4 | 1 | 0 | 81.19 |
| 1.158 | 10 | 4 | 1 | 1 | 83.39 |
| 1.156 | 4 | 4 | 0 | 2 | 83.61 |
| 1.153 | 8 | 3 | 2 | 1 | 83.88 |
| 1.108 | 2 | 2 | 2 | 3 | 88.12 |
| 1.091 | 7 | 1 | 0 | 5 | 89.80 |
| 1.090 | 1 | 4 | 1 | 2 | 89.94 |
| 1.073 | 2 | 0 | 3 | 1 | 91.73 |
| 1.058 | 1 | 0 | 1 | 5 | 93.48 |
| 1.050 | 2 | 1 | 3 | 1 | 94.37 |
| 1.049 | 2 | 4 | 0 | 3 | 94.52 |
| 1.041 | 2 | 1 | 2 | 4 | 95.47 |
| 1.036 | 2 | 1 | 1 | 5 | 96.13 |
| 1.023 | 18 | 3 | 1 | 4 | 97.64 |
| 1.004 | 1 | 2 | 3 | 0 | 100.16 |
| 1.004 | 5 | 4 | 2 | 0 | 100.23 |
| .999 | 3 | 4 | 1 | 3 | 100.90 |
| .999 | 5 | 1 | 3 | 2 | 100.97 |
| .995 | 5 | 3 | 2 | 3 | 101.39 |
| .989 | 11 | 2 | 3 | 1 | 102.38 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .988 | 1 | 4 | 2 | 1 | 102.45 |
| .981 | 2 | 2 | 2 | 4 | 103.50 |
| .945 | 4 | 4 | 2 | 2 | 109.25 |
| .943 | 6 | 0 | 3 | 3 | 109.53 |
| .932 | 1 | 3 | 0 | 5 | 111.40 |
| .916 | 10 | 5 | 1 | 2 | 114.41 |
| .909 | 11 | 1 | 2 | 5 | 115.94 |
| .891 | 3 | 5 | 0 | 3 | 119.55 |
| .884 | 3 | 4 | 2 | 3 | 121.32 |
| .882 | 7 | 1 | 1 | 6 | 121.66 |
| .874 | 3 | 2 | 0 | 6 | 123.56 |
| .8490 | 5 | 1 | 3 | 4 | 130.28 |
| .8462 | 4 | 6 | 0 | 0 | 131.10 |
| .8447 | 2 | 2 | 1 | 6 | 131.53 |
| .8285 | 2 | 4 | 3 | 0 | 136.79 |
| .8202 | 7 | 0 | 4 | 0 | 139.80 |
| .8196 | 8 | 4 | 3 | 1 | 140.07 |
| .8194 | 2 | 6 | 1 | 0 | 140.15 |
| .8107 | 6 | 6 | 1 | 1 | 143.68 |
| .8107 | 3 | 3 | 2 | 5 | 143.68 |
| .8098 | 2 | 6 | 0 | 2 | 144.05 |
| .7967 | 2 | 5 | 1 | 4 | 150.40 |
| .7943 | 2 | 4 | 3 | 2 | 151.75 |
| .7917 | 11 | 3 | 1 | 6 | 153.28 |
| .7885 | 2 | 1 | 0 | 7 | 155.36 |
| .7870 | 2 | 0 | 4 | 2 | 156.33 |
| .7862 | 1 | 6 | 1 | 2 | 156.89 |
| .7833 | 13 | 5 | 2 | 3 | 159.09 |

# Cobalt phosphide, $CoP_3$

Structure
Cubic, Im3 (204), Z = 8, isostructural with $CoAs_3$, from powder data [Rundqvist and Ersson, 1968]. Munson and Kasper [1968] reported a high pressure phase deficient in cobalt, with a similar cell.

Atom positions [Rundqvist and Ersson, 1968]
8(c) 8 cobalt
24(g) 24 phosphorus

Lattice constant
a = 7.7078 A
(published value, 7.7073 Å [Rundqvist and Ersson, 1968]).

Volume
457.92 $Å^3$

Density
(calculated) 4.404 $g/cm^3$

Thermal parameters
Isotropic [Rundqvist and Ersson, 1968].

Scattering factors
$Co^0$, $P^0$ [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 0.196 \times 10^{-3}$


References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Munson, R. A. and Kasper, J. S.(1968). Inorg. Chem. 7, 390.
Rundqvist, S. and Ersson, N. (1968). Ark. Kemi 30, 103.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 5.447 | 25 | 1 1 0 | 16.26 |
| 3.8538 | 100 | 2 0 0 | 23.06 |
| 3.1467 | 15 | 2 1 1 | 28.34 |
| 2.7250 | 65 | 2 2 0 | 32.84 |
| 2.4365 | 100 | 0 1 3 | 36.86 |
| 2.2245 | 30 | 2 2 2 | 40.52 |
| 2.0598 | 25 | 1 2 3 | 43.92 |
| 1.9271 | 8 | 4 0 0 | 47.12 |
| 1.8166 | 6 | 3 3 0+ | 50.18 |
| 1.7233 | 90 | 4 2 0+ | 53.10 |
| 1.6435 | 6 | 3 3 2 | 55.90 |
| 1.5735 | 50 | 4 2 2 | 58.62 |
| 1.5115 | 25 | 4 3 1+ | 61.28 |
| 1.3624 | 2 | 4 4 0 | 68.86 |
| 1.3220 | 7 | 4 3 3+ | 71.28 |
| 1.2847 | 2 | 4 4 2 | 73.68 |
| 1.2188 | 13 | 0 2 6+ | 78.40 |
| 1.1892 | 1 | 1 4 5+ | 80.74 |
| 1.1620 | 11 | 6 2 2 | 83.04 |
| 1.1365 | 7 | 1 3 6 | 85.34 |
| 1.1125 | 10 | 4 4 4 | 87.64 |
| 1.0901 | 2 | 3 4 5+ | 89.92 |
| 1.0689 | 11 | 6 4 0+ | 92.22 |
| 1.0488 | 3 | 6 3 3+ | 94.52 |
| 1.0299 | 5 | 2 4 6+ | 96.82 |
| 1.0121 | 6 | 7 3 0 | 99.12 |
| .9789 | 4 | 2 3 7+ | 103.80 |
| .9635 | 4 | 8 0 0 | 106.16 |
| .9488 | 1 | 1 4 7+ | 108.56 |
| .9347 | 11 | 6 4 4+ | 111.00 |
| .9213 | 1 | 3 5 6+ | 113.46 |
| .9084 | 12 | 6 6 0+ | 115.98 |
| .8960 | 11 | 7 4 3+ | 118.56 |
| .8842 | 3 | 6 6 2 | 121.20 |
| .8618 | 1 | 8 4 0+ | 126.72 |
| .8512 | 2 | 0 1 9+ | 129.64 |
| .8410 | 7 | 2 4 8+ | 132.68 |
| .8311 | 1 | 7 6 1+ | 135.88 |
| .8216 | 1 | 6 6 4 | 139.28 |
| .8125 | 1 | 4 5 7+ | 142.92 |
| .7950 | 6 | 3 6 7+ | 151.36 |
| .7867 | 4 | 8 4 4 | 156.58 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 5.450 | 20 | 1 | 1 | 0 | 16.25 |
| 3.8539 | 100 | 2 | 0 | 0 | 23.06 |
| 3.1467 | 16 | 2 | 1 | 1 | 28.34 |
| 2.7251 | 70 | 2 | 2 | 0 | 32.84 |
| 2.4374 | 18 | 3 | 1 | 0 | 36.85 |
| 2.4374 | 95 | 0 | 1 | 3 | 36.85 |
| 2.2251 | 35 | 2 | 2 | 2 | 40.51 |
| 2.0600 | 25 | 1 | 2 | 3 | 43.92 |
| 1.9270 | 10 | 4 | 0 | 0 | 47.13 |
| 1.8167 | 5 | 3 | 3 | 0 | 50.17 |
| 1.8167 | 2 | 4 | 1 | 1 | 50.17 |
| 1.7235 | 60 | 4 | 2 | 0 | 53.09 |
| 1.7235 | 50 | 0 | 2 | 4 | 53.09 |
| 1.6433 | 7 | 3 | 3 | 2 | 55.91 |
| 1.5733 | 60 | 4 | 2 | 2 | 58.63 |
| 1.5116 | 25 | 4 | 3 | 1 | 61.27 |
| 1.5116 | 2 | 5 | 1 | 0 | 61.27 |
| 1.5116 | 2 | 0 | 1 | 5 | 61.27 |
| 1.5116 | 5 | 1 | 3 | 4 | 61.27 |
| 1.3626 | 3 | 4 | 4 | 0 | 68.85 |
| 1.3219 | 2 | 5 | 3 | 0 | 71.29 |
| 1.3219 | 5 | 4 | 3 | 3 | 71.29 |
| 1.3219 | 3 | 0 | 3 | 5 | 71.29 |
| 1.2846 | 3 | 4 | 4 | 2 | 73.69 |
| 1.2187 | 8 | 6 | 2 | 0 | 78.40 |
| 1.2187 | 9 | 0 | 2 | 6 | 78.40 |
| 1.1893 | 1 | 1 | 4 | 5 | 80.73 |
| 1.1620 | 15 | 6 | 2 | 2 | 83.04 |
| 1.1365 | 1 | 6 | 3 | 1 | 85.35 |
| 1.1365 | 8 | 1 | 3 | 6 | 85.35 |
| 1.1125 | 13 | 4 | 4 | 4 | 87.64 |
| 1.0900 | 1 | 5 | 4 | 3 | 89.93 |
| 1.0900 | 1 | 0 | 1 | 7 | 89.93 |
| 1.0900 | 1 | 3 | 4 | 5 | 89.93 |
| 1.0689 | 8 | 6 | 4 | 0 | 92.22 |
| 1.0689 | 7 | 0 | 4 | 6 | 92.22 |
| 1.0489 | 2 | 6 | 3 | 3 | 94.51 |
| 1.0489 | 1 | 1 | 2 | 7 | 94.51 |
| 1.0300 | 2 | 6 | 4 | 2 | 96.81 |
| 1.0300 | 4 | 2 | 4 | 6 | 96.81 |
| 1.0121 | 8 | 7 | 3 | 0 | 99.12 |
| 1.0121 | 1 | 0 | 3 | 7 | 99.12 |
| .9789 | 4 | 2 | 3 | 7 | 103.80 |
| .9635 | 6 | 8 | 0 | 0 | 106.16 |
| .9488 | 1 | 1 | 4 | 7 | 108.56 |
| .9347 | 2 | 8 | 2 | 0 | 111.00 |
| .9347 | 4 | 0 | 2 | 8 | 111.00 |
| .9347 | 10 | 6 | 4 | 4 | 111.00 |
| .9213 | 2 | 3 | 5 | 6 | 113.47 |
| .9084 | 14 | 6 | 6 | 0 | 115.99 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .9084 | 5 | 8 | 2 | 2 | 115.99 |
| .8960 | 1 | 0 | 5 | 7 | 118.56 |
| .8960 | 1 | 7 | 5 | 0 | 118.56 |
| .8960 | 2 | 1 | 3 | 8 | 118.56 |
| .8960 | 11 | 7 | 4 | 3 | 118.56 |
| .8960 | 1 | 3 | 4 | 7 | 118.56 |
| .8841 | 5 | 6 | 6 | 2 | 121.21 |
| .8618 | 2 | 8 | 4 | 0 | 126.73 |
| .8512 | 2 | 0 | 1 | 9 | 129.64 |
| .8410 | 8 | 8 | 4 | 2 | 132.68 |
| .8410 | 8 | 2 | 4 | 8 | 132.68 |
| .8312 | 1 | 7 | 6 | 1 | 135.88 |
| .8312 | 1 | 1 | 2 | 9 | 135.88 |
| .8217 | 3 | 6 | 6 | 4 | 139.27 |
| .8125 | 1 | 7 | 5 | 4 | 142.92 |
| .8125 | 2 | 4 | 5 | 7 | 142.92 |
| .7950 | 2 | 9 | 3 | 2 | 151.36 |
| .7950 | 16 | 3 | 6 | 7 | 151.36 |
| .7867 | 12 | 8 | 4 | 4 | 156.58 |

# Cobalt plutonium, $CoPu_2$

Structure
Hexagonal, $P\bar{6}2m$ (189), Z = 3, cobalt-rich end member, isostructural with $Fe_2P$, from powder data [Ellinger, 1961].

Atom positions
The positions were assigned by comparisons of cell edge and atomic radii ratios; the positions for $Ni_6Si_2P$ [Rundqvist and Jellinek, 1959] were preferred to those for $Fe_2P$, for this cobalt-rich end member.

| | | | |
|---|---|---|---|
| 3(f) | 3 pluto ium | 2(c) | 2 cobalt |
| 3(g) | 3 plutonium | 1(b) | 1 cobalt |

Lattice constants [Ellinger, 1961]
a = 7.763 A
c = 3.648

Volume
190.4 $A^3$

Density
(calculated) 14.21 $g/cm^3$

Thermal parameters
Isotropic: plutonium, B = 0.4
cobalt, B = 0.52, the value for nickel, used by Rundqvist and Jellinek [1959].

Scattering factors
$Co^0$, $Pu^0$ [International Tables, 1962], corrected for anomalous dispersion [Dauben and Templeton, 1955].

Scale factor (integrated intensities)
$\gamma = 0.707 \times 10^{-3}$

References


Dauben, C. H. and Templeton, D. H. (1955). Acta Crystallogr. 8, 241.

Ellinger, F. H. (1961). The Metal Plutonium. World Metallurgical Congress, 1957 (Univ. of Chicago Press, Chicago) p. 288.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, England) pp. 204, 212.

Rundqvist, S. and Jellinek, F. (1959). Acta Chem. Scand. 13, 425.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 6.72 | 7 | 1 0 0 | 13.16 |
| 3.880 | 16 | 1 1 0 | 22.90 |
| 3.361 | 1 | 2 0 0 | 26.50 |
| 3.207 | 9 | 1 0 1 | 27.80 |
| 2.657 | 100 | 1 1 1 | 33.70 |
| 2.541 | 60 | 2 1 0 | 35.30 |
| 2.472 | 40 | 2 0 1 | 36.32 |
| 2.240 | 20 | 3 0 0 | 40.22 |
| 2.085 | 15 | 2 1 1 | 43.36 |
| 1.940 | 3 | 2 2 0 | 46.78 |
| 1.910 | 1 | 3 0 1 | 47.58 |
| 1.865 | 6 | 3 1 0 | 48.80 |
| 1.824 | 12 | 0 0 2 | 49.96 |
| 1.713 | 2 | 2 2 1 | 53.44 |
| 1.681 | 3 | 4 0 0 | 54.56 |
| 1.660 | 15 | 3 1 1 | 55.28 |
| 1.651 | 3 | 1 1 2 | 55.62 |
| 1.542 | 4 | 3 2 0 | 59.92 |
| 1.526 | 8 | 4 0 1 | 60.62 |
| 1.482 | 17 | 2 1 2 | 62.64 |
| 1.467 | 2 | 4 1 0 | 63.34 |
| 1.420 | 16 | 3 2 1 | 65.68 |
| 1.415 | 10 | 3 0 2 | 65.98 |
| 1.361 | 5 | 4 1 1 | 68.94 |
| 1.345 | 4 | 5 0 0 | 69.90 |
| 1.329 | 2 | 2 2 2 | 70.84 |
| 1.304 | 3 | 3 1 2 | 72.42 |
| 1.294 | 2 | 3 3 0 | 73.08 |
| 1.271 | 4 | 4 2 0 | 74.64 |
| 1.262 | 2 | 5 0 1 | 75.26 |
| 1.236 | 2 | 4 0 2 | 77.10 |
| 1.219 | 1 | 3 3 1 | 78.36 |
| 1.207 | 2 | 5 1 0 | 79.28 |
| 1.200 | 4 | 4 2 1 | 79.88 |
| 1.178 | 3 | 3 2 2 | 81.70 |
| 1.160 | 5 | 1 1 3 | 83.18 |
| 1.146 | 2 | 5 1 1 | 84.44 |
| 1.143 | 4 | 2 0 3+ | 84.70 |
| 1.097 | 1 | 2 1 3 | 89.22 |
| 1.082 | 4 | 5 0 2 | 90.76 |
| 1.076 | 1 | 5 2 0 | 91.38 |
| 1.058 | 1 | 4 3 1 | 93.48 |
| 1.055 | 3 | 3 3 2 | 93.76 |
| 1.042 | 4 | 4 2 2 | 95.28 |
| 1.032 | 3 | 5 2 1 | 96.50 |
| 1.025 | 1 | 6 1 0 | 97.42 |
| 1.018 | 3 | 3 1 3 | 98.28 |
| 1.007 | 3 | 5 1 2 | 99.82 |
| .987 | 8 | 6 1 1 | 102.60 |
| .985 | 5 | 4 0 3 | 102.96 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .970 | 1 | 4 | 4 | 0 | 105.08 |
| .960 | 2 | 5 | 3 | 0 | 106.66 |
| .955 | 5 | 3 | 2 | 3 | 107.54 |
| .945 | 1 | 4 | 3 | 2 | 109.16 |
| .938 | 4 | 4 | 4 | 1 | 110.46 |
| .936 | 2 | 4 | 1 | 3 | 110.74 |
| .929 | 1 | 5 | 3 | 1 | 112.08 |
| .927 | 2 | 5 | 2 | 2 | 112.38 |
| .912 | 1 | 0 | 0 | 4 | 115.26 |
| .903 | 1 | 6 | 2 | 1 | 117.04 |
| .902 | 1 | 5 | 0 | 3 | 117.32 |
| .894 | 2 | 6 | 1 | 2 | 119.06 |
| .891 | 1 | 7 | 1 | 0 | 119.76 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 6.72 | 6 | 1 | 0 | 0 | 13.16 |
| 3.882 | 15 | 1 | 1 | 0 | 22.89 |
| 3.361 | 1 | 2 | 0 | 0 | 26.49 |
| 3.206 | 9 | 1 | 0 | 1 | 27.80 |
| 2.658 | 100 | 1 | 1 | 1 | 33.69 |
| 2.541 | 60 | 2 | 1 | 0 | 35.29 |
| 2.472 | 40 | 2 | 0 | 1 | 36.31 |
| 2.241 | 25 | 3 | 0 | 0 | 40.21 |
| 2.085 | 16 | 2 | 1 | 1 | 43.36 |
| 1.941 | 3 | 2 | 2 | 0 | 46.77 |
| 1.909 | 1 | 3 | 0 | 1 | 47.58 |
| 1.865 | 7 | 3 | 1 | 0 | 48.80 |
| 1.824 | 14 | 0 | 0 | 2 | 49.96 |
| 1.713 | 3 | 2 | 2 | 1 | 53.43 |
| 1.681 | 3 | 4 | 0 | 0 | 54.56 |
| 1.660 | 17 | 3 | 1 | 1 | 55.28 |
| 1.651 | 3 | 1 | 1 | 2 | 55.63 |
| 1.542 | 5 | 3 | 2 | 0 | 59.92 |
| 1.527 | 10 | 4 | 0 | 1 | 60.61 |
| 1.482 | 20 | 2 | 1 | 2 | 62.64 |
| 1.467 | 1 | 4 | 1 | 0 | 63.34 |
| 1.421 | 19 | 3 | 2 | 1 | 65.67 |
| 1.415 | 9 | 3 | 0 | 2 | 65.98 |
| 1.361 | 6 | 4 | 1 | 1 | 68.93 |
| 1.345 | 5 | 5 | 0 | 0 | 69.90 |
| 1.329 | 2 | 2 | 2 | 2 | 70.84 |
| 1.304 | 4 | 3 | 1 | 2 | 72.42 |
| 1.294 | 2 | 3 | 3 | 0 | 73.08 |
| 1.271 | 5 | 4 | 2 | 0 | 74.64 |
| 1.262 | 2 | 5 | 0 | 1 | 75.26 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.236 | 2 | 4 | 0 | 2 | 77.10 |
| 1.219 | 1 | 3 | 3 | 1 | 78.35 |
| 1.207 | 3 | 5 | 1 | 0 | 79.28 |
| 1.200 | 4 | 4 | 2 | 1 | 79.88 |
| 1.178 | 4 | 3 | 2 | 2 | 81.70 |
| 1.160 | 6 | 1 | 1 | 3 | 83.18 |
| 1.146 | 2 | 5 | 1 | 1 | 84.44 |
| 1.143 | 3 | 2 | 0 | 3 | 84.70 |
| 1.143 | 1 | 4 | 1 | 2 | 84.73 |
| 1.105 | 1 | 4 | 3 | 0 | 88.37 |
| 1.097 | 2 | 2 | 1 | 3 | 89.22 |
| 1.082 | 5 | 5 | 0 | 2 | 90.75 |
| 1.077 | 2 | 5 | 2 | 0 | 91.37 |
| 1.058 | 1 | 4 | 3 | 1 | 93.48 |
| 1.055 | 3 | 3 | 3 | 2 | 93.76 |
| 1.043 | 5 | 4 | 2 | 2 | 95.27 |
| 1.033 | 4 | 5 | 2 | 1 | 96.50 |
| 1.025 | 2 | 6 | 1 | 0 | 97.41 |
| 1.019 | 4 | 3 | 1 | 3 | 98.27 |
| 1.007 | 4 | 5 | 1 | 2 | 99.82 |
| .987 | 10 | 6 | 1 | 1 | 102.60 |
| .985 | 3 | 4 | 0 | 3 | 102.87 |
| .970 | 1 | 4 | 4 | 0 | 105.09 |
| .960 | 2 | 5 | 3 | 0 | 106.65 |
| .955 | 6 | 3 | 2 | 3 | 107.54 |
| .945 | 1 | 4 | 3 | 2 | 109.16 |
| .938 | 5 | 4 | 4 | 1 | 110.45 |
| .936 | 2 | 4 | 1 | 3 | 110.73 |
| .929 | 1 | 5 | 3 | 1 | 112.07 |
| .927 | 3 | 5 | 2 | 2 | 112.38 |
| .912 | 2 | 0 | 0 | 4 | 115.26 |
| .903 | 2 | 6 | 2 | 1 | 117.03 |
| .902 | 1 | 5 | 0 | 3 | 117.32 |
| .894 | 3 | 6 | 1 | 2 | 119.06 |
| .890 | 1 | 7 | 1 | 0 | 119.77 |

# Cobalt plutonium, $CoPu_6$

Structure
Tetragonal, I4/mcm (140), Z = 4, isostructural with $MnU_6$, from powder data [Ellinger, 1961].

Atom positions
The positions and distributions of $MnU_6$ were used [Baenziger et al., 1950]

Lattice constants
[Poole et al., 1961, Table 6.1]
a = 10.476 A
c = 5.340
(published values: a = 10.475, c = 5.340 Å)

Volume
586.1 $Å^3$

Density
(calculated) 17.12 $g/cm^3$

Thermal parameters
Isotropic: cobalt, B = 1.0; plutonium, B = 0.75

Scattering factors
$Co^0$, $Pu^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 2.67 \times 10^{-3}$

References


Baenziger, N. C., Rundle, R. E., Snow, A. I., and Wilson, A. S. (1950). Acta Crystallogr. 3, 34.

Ellinger, F. H. (1961). The Metal Plutonium. World Metallurgical Conference, 1957, (Univ. of Chicago Press, Chicago) p. 288

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England). pp. 204, 212.

Poole, D.M., Bale, M. G., Mardon, P. G., Marples, J. A. C., and Nichols, J. C. (1961). Plutonium 1960. International Conference on Plutonium Metallurgy, (2nd) Cleaver Hume Press, London). p. 276.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 7.41 | 4 | 1 1 0 | 11.94 |
| 3.70 | 1 | 2 2 0 | 24.02 |
| 3.52 | 2 | 2 1 1 | 25.28 |
| 3.31 | 2 | 3 1 0 | 26.90 |
| 2.670 | 30 | 0 0 2 | 33.54 |
| 2.618 | 5 | 4 0 0 | 34.22 |
| 2.552 | 100 | 3 2 1 | 35.14 |
| 2.512 | 4 | 1 1 2 | 35.72 |
| 2.469 | 2 | 3 3 0 | 36.36 |
| 2.378 | 1 | 2 0 2 | 37.80 |
| 2.342 | 6 | 4 2 0 | 38.40 |
| 2.294 | 6 | 4 1 1 | 39.24 |
| 2.166 | 2 | 2 2 2 | 41.66 |
| 2.079 | 4 | 3 1 2 | 43.50 |
| 2.055 | 12 | 5 1 0 | 44.04 |
| 1.951 | 2 | 4 3 1 | 46.52 |
| 1.870 | 5 | 4 0 2 | 48.66 |
| 1.761 | 2 | 4 2 2 | 51.88 |
| 1.746 | 5 | 6 0 0 | 52.36 |
| 1.639 | 6 | 6 1 1 | 56.06 |
| 1.628 | 7 | 5 1 2 | 56.48 |
| 1.518 | 17 | 3 2 3 | 61.00 |
| 1.481 | 6 | 5 5 0 | 62.66 |
| 1.461 | 7 | 6 0 2 | 63.62 |
| 1.458 | 5 | 4 1 3 | 63.80 |
| 1.389 | 4 | 7 2 1 | 67.34 |
| 1.335 | 3 | 0 0 4 | 70.48 |
| 1.295 | 9 | 5 5 2 | 72.98 |
| 1.238 | 2 | 6 1 3 | 76.98 |
| 1.235 | 2 | 6 6 0 | 77.20 |
| 1.195 | 11 | 8 3 1 | 80.28 |
| 1.160 | 1 | 4 2 4 | 83.24 |
| 1.119 | 4 | 5 1 4+ | 86.98 |
| 1.111 | 1 | 7 6 1+ | 87.76 |
| 1.061 | 2 | 6 0 4 | 93.16 |
| 1.048 | 2 | 10 0 0 | 94.66 |
| 1.021 | 1 | 9 3 2 | 98.02 |
| 1.010 | 7 | 8 3 3 | 99.44 |
| 1.002 | 4 | 3 2 5 | 100.42 |
| .992 | 3 | 5 5 4 | 101.92 |
| .975 | 3 | 10 0 2 | 104.34 |
| .969 | 3 | 8 7 1 | 105.28 |
| .958 | 1 | 7 6 3+ | 107.08 |

Cobalt plutonium, $CoPu_6$ - (continued)

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 7.41 | 3 | 1 | 1 | 0 | 11.94 |
| 3.70 | 1 | 2 | 2 | 0 | 24.01 |
| 3.52 | 2 | 2 | 1 | 1 | 25.27 |
| 3.31 | 2 | 3 | 1 | 0 | 26.89 |
| 2.670 | 25 | 0 | 0 | 2 | 33.54 |
| 2.619 | 4 | 4 | 0 | 0 | 34.21 |
| 2.552 | 100 | 3 | 2 | 1 | 35.13 |
| 2.512 | 2 | 1 | 1 | 2 | 35.72 |
| 2.469 | 2 | 3 | 3 | 0 | 36.35 |
| 2.379 | 1 | 2 | 0 | 2 | 37.79 |
| 2.343 | 6 | 4 | 2 | 0 | 38.40 |
| 2.294 | 6 | 4 | 1 | 1 | 39.24 |
| 2.166 | 2 | 2 | 2 | 2 | 41.67 |
| 2.079 | 4 | 3 | 1 | 2 | 43.50 |
| 2.055 | 13 | 5 | 1 | 0 | 44.04 |
| 1.950 | 2 | 4 | 3 | 1 | 46.52 |
| 1.870 | 5 | 4 | 0 | 2 | 48.66 |
| 1.761 | 2 | 4 | 2 | 2 | 51.88 |
| 1.746 | 6 | 6 | 0 | 0 | 52.36 |
| 1.639 | 6 | 6 | 1 | 1 | 56.06 |
| 1.628 | 8 | 5 | 1 | 2 | 56.47 |
| 1.522 | 1 | 4 | 4 | 2 | 60.82 |
| 1.518 | 19 | 3 | 2 | 3 | 61.00 |
| 1.482 | 7 | 5 | 5 | 0 | 62.66 |
| 1.461 | 8 | 6 | 0 | 2 | 63.62 |
| 1.458 | 1 | 4 | 1 | 3 | 63.79 |
| 1.389 | 5 | 7 | 2 | 1 | 67.34 |
| 1.335 | 3 | 0 | 0 | 4 | 70.48 |
| 1.295 | 10 | 5 | 5 | 2 | 72.97 |
| 1.238 | 2 | 6 | 1 | 3 | 76.98 |
| 1.235 | 1 | 6 | 6 | 0 | 77.21 |
| 1.195 | 13 | 8 | 3 | 1 | 80.27 |
| 1.160 | 1 | 4 | 2 | 4 | 83.23 |
| 1.121 | 1 | 6 | 6 | 2 | 86.85 |
| 1.119 | 3 | 5 | 1 | 4 | 86.96 |
| 1.119 | 2 | 7 | 2 | 3 | 87.00 |
| 1.061 | 2 | 6 | 0 | 4 | 93.16 |
| 1.048 | 2 | 10 | 0 | 0 | 94.66 |
| 1.020 | 1 | 9 | 3 | 2 | 98.03 |
| 1.010 | 8 | 8 | 3 | 3 | 99.43 |
| 1.002 | 5 | 3 | 2 | 5 | 100.43 |
| .992 | 4 | 5 | 5 | 4 | 101.92 |
| .975 | 3 | 10 | 0 | 2 | 104.35 |
| .969 | 4 | 8 | 7 | 1 | 105.28 |

# Cobalt plutonium, $Co_2Pu$

Structure
Cubic, Fd3m (227), Z = 8, isostructural with $Cu_2Mg$, from powder data [Ellinger, 1961]. Their sample was described as plutonium-rich.

Atom positions
8(a) 8 plutonium
16(d) 16 cobalt
The origin was taken at $\bar{4}3m$.

Lattice constant
a = 7.081 A [Ellinger, 1961].

Volume
355.1 $Å^3$

Density
(calculated) 13.462 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$ [Cromer and Mann, 1968]
$Pu^0$ [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 1.370 \times 10^{-3}$


References
Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.
Ellinger, F. H. (1961). In The Metal Plutonium, (Univ. of Chicago Press, Chicago). World Metallurgical Conference, 1957 (edited by Coffinberry, A. S. and Miner, W. N.) p. 288.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.08 | 45 | 1 1 1 | 21.74 |
| 2.504 | 90 | 2 2 0 | 35.84 |
| 2.135 | 100 | 3 1 1 | 42.30 |
| 2.044 | 10 | 2 2 2 | 44.28 |
| 1.771 | 5 | 4 0 0 | 51.58 |
| 1.624 | 10 | 3 3 1 | 56.62 |
| 1.446 | 25 | 4 2 2 | 64.40 |
| 1.363 | 25 | 5 1 1+ | 68.84 |
| 1.252 | 15 | 4 4 0 | 75.96 |
| 1.197 | 5 | 5 3 1 | 80.12 |
| 1.120 | 10 | 6 2 0 | 86.94 |
| 1.080 | 5 | 5 3 3 | 91.02 |
| 1.067 | 1 | 6 2 2 | 92.38 |
| 1.022 | 1 | 4 4 4 | 97.82 |
| .991 | 5 | 7 1 1+ | 101.96 |
| .946 | 10 | 6 4 2 | 109.00 |
| .922 | 15 | 7 3 1+ | 113.36 |
| .885 | 5 | 8 0 0 | 120.98 |
| .865 | 1 | 7 3 3 | 125.86 |
| .834 | 5 | 8 2 2+ | 134.76 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.09 | 40 | 1 1 1 | 21.72 |
| 2.504 | 85 | 2 2 0 | 35.84 |
| 2.135 | 100 | 3 1 1 | 42.30 |
| 2.044 | 10 | 2 2 2 | 44.28 |
| 1.770 | 5 | 4 0 0 | 51.59 |
| 1.624 | 10 | 3 3 1 | 56.61 |
| 1.445 | 30 | 4 2 2 | 64.41 |
| 1.363 | 20 | 5 1 1 | 68.84 |
| 1.363 | 5 | 3 3 3 | 68.84 |
| 1.252 | 20 | 4 4 0 | 75.96 |
| 1.197 | 5 | 5 3 1 | 80.12 |
| 1.120 | 10 | 6 2 0 | 86.95 |
| 1.080 | 10 | 5 3 3 | 91.02 |
| 1.068 | 1 | 6 2 2 | 92.37 |
| 1.022 | 1 | 4 4 4 | 97.82 |
| .992 | 1 | 7 1 1 | 101.95 |
| .992 | 1 | 5 5 1 | 101.95 |
| .946 | 15 | 6 4 2 | 108.99 |
| .922 | 15 | 7 3 1 | 113.35 |
| .922 | 5 | 5 5 3 | 113.35 |
| .885 | 5 | 8 0 0 | 120.98 |
| .865 | 1 | 7 3 3 | 125.86 |
| .835 | 10 | 8 2 2 | 134.76 |
| .835 | 5 | 6 6 0 | 134.76 |
| .818 | 15 | 7 5 1 | 140.81 |

# Cobalt plutonium, $Co_3Pu$

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 9, isostructural with $Ni_3Pu$, from powder data [Poole et al., 1961].

Atom positions
The positions assumed were those refined for $Ni_3Pu$ [Cromer and Olsen, 1959].

Lattice constants [Poole et al., 1961]
a = 5.003 Å
c = 24.42

Volume
529.3 $Å^3$

Density
(calculated) 11.82 $g/cm^3$

Thermal parameters
Isotropic values were used from Cromer and Olsen [1959], with their data for nickel applied to the cobalt atoms here.

Scattering factors
$Co^0$, $Pu^0$ [International Tables, 1962], corrected for anomalous dispersion [Cromer and Olsen, 1959].

Scale factor (integrated intensities)
$\gamma = 0.369 \times 10^{-3}$


References
Cromer, D. T. and Olsen, C. E. (1959). Acta Crystallogr. 12, 689.
International Tables for X-ray Crystallography, III, (The Kynoch Press, Birmingham, England), pp. 202,204.
Poole, D. M., Bale, M. G., Marden, P. G., Marples, J. A. C., and Nichols, J. L. (1961). In Plutonium, 1960 (Cleaver Hume Press, London). International Conference on Plutonium Metallurgy, (2nd). Edited by Grison, E., Lord, W. B. H., and Fowler, R. D., p. 267.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 8.14 | 8 | 0 0 3 | 10.86 |
| 4.26 | 35 | 1 0 1 | 20.82 |
| 4.07 | 14 | 0 0 6 | 21.82 |
| 3.531 | 5 | 1 0 4 | 25.20 |
| 3.241 | 2 | 0 1 5 | 27.50 |
| 2.717 | 65 | 1 0 7 | 32.94 |
| 2.501 | 80 | 1 1 0 | 35.88 |
| 2.495 | 85 | 0 1 8 | 35.96 |
| 2.391 | 2 | 1 1 3 | 37.58 |
| 2.157 | 35 | 0 2 1 | 41.84 |
| 2.131 | 100 | 1 1 6 | 42.38 |
| 2.041 | 10 | 0 2 4 | 44.34 |
| 2.035 | 13 | 0 0 12 | 44.48 |
| 1.975 | 14 | 0 1 11+ | 45.90 |
| 1.839 | 6 | 1 1 9+ | 49.52 |
| 1.767 | 4 | 2 0 8 | 51.70 |
| 1.723 | 2 | 1 0 13 | 53.10 |
| 1.634 | 4 | 2 1 1 | 56.26 |
| 1.628 | 5 | 0 0 15 | 56.48 |
| 1.618 | 10 | 0 1 14 | 56.86 |
| 1.581 | 1 | 2 1 4 | 58.30 |
| 1.578 | 2 | 1 1 12 | 58.42 |
| 1.482 | 15 | 2 1 7 | 62.62 |
| 1.444 | 17 | 1 2 8+ | 64.50 |
| 1.419 | 7 | 0 2 13 | 65.74 |
| 1.364 | 12 | 1 1 15 | 68.74 |
| 1.361 | 25 | 3 0 6+ | 68.94 |
| 1.359 | 18 | 2 0 14 | 69.08 |
| 1.318 | 4 | 1 2 11 | 71.54 |
| 1.2749 | 1 | 0 3 9+ | 74.34 |
| 1.2506 | 13 | 2 2 0 | 76.04 |
| 1.2344 | 1 | 2 1 13 | 77.22 |
| 1.2001 | 2 | 1 3 1 | 79.86 |
| 1.1971 | 4 | 2 0 17 | 80.10 |
| 1.1939 | 8 | 1 2 14 | 80.36 |
| 1.1753 | 2 | 0 1 20 | 81.90 |
| 1.1630 | 1 | 0 0 21 | 82.96 |
| 1.1361 | 6 | 1 3 7 | 85.38 |
| 1.1182 | 4 | 3 1 8 | 87.08 |
| 1.1154 | 3 | 2 1 16 | 87.36 |
| 1.1053 | 1 | 0 2 19 | 88.36 |
| 1.0820 | 3 | 4 0 1 | 90.78 |
| 1.0804 | 5 | 3 0 15+ | 90.96 |
| 1.0754 | 2 | 1 0 22 | 91.50 |
| 1.0656 | 4 | 2 2 12 | 92.58 |
| 1.0569 | 2 | 3 1 11 | 93.58 |
| 1.0545 | 7 | 1 1 21 | 93.86 |
| 1.0208 | 1 | 0 4 8 | 97.98 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 8.14 | 7 | 0 | 0 | 3 | 10.86 |
| 4.27 | 30 | 1 | 0 | 1 | 20.81 |
| 4.08 | 2 | 0 | 1 | 2 | 21.75 |
| 4.07 | 12 | 0 | 0 | 6 | 21.82 |
| 3.533 | 4 | 1 | 0 | 4 | 25.18 |
| 3.241 | 2 | 0 | 1 | 5 | 27.50 |
| 2.717 | 65 | 1 | 0 | 7 | 32.94 |
| 2.713 | 3 | 0 | 0 | 9 | 32.99 |
| 2.502 | 70 | 1 | 1 | 0 | 35.87 |
| 2.495 | 45 | 0 | 1 | 8 | 35.96 |
| 2.391 | 2 | 1 | 1 | 3 | 37.59 |
| 2.158 | 40 | 0 | 2 | 1 | 41.83 |
| 2.133 | 8 | 2 | 0 | 2 | 42.34 |
| 2.131 | 100 | 1 | 1 | 6 | 42.38 |
| 2.127 | 4 | 1 | 0 | 10 | 42.46 |
| 2.042 | 9 | 0 | 2 | 4 | 44.33 |
| 2.035 | 10 | 0 | 0 | 12 | 44.48 |
| 1.980 | 8 | 2 | 0 | 5 | 45.78 |
| 1.976 | 11 | 0 | 1 | 11 | 45.89 |
| 1.840 | 2 | 0 | 2 | 7 | 49.49 |
| 1.839 | 5 | 1 | 1 | 9 | 49.52 |
| 1.767 | 4 | 2 | 0 | 8 | 51.70 |
| 1.723 | 2 | 1 | 0 | 13 | 53.10 |
| 1.634 | 4 | 2 | 1 | 1 | 56.25 |
| 1.628 | 4 | 0 | 0 | 15 | 56.48 |
| 1.618 | 11 | 0 | 1 | 14 | 56.86 |
| 1.582 | 1 | 2 | 1 | 4 | 58.29 |
| 1.579 | 1 | 1 | 1 | 12 | 58.41 |
| 1.482 | 18 | 2 | 1 | 7 | 62.61 |
| 1.444 | 11 | 3 | 0 | 0 | 64.47 |
| 1.443 | 14 | 1 | 2 | 8 | 64.52 |
| 1.440 | 1 | 1 | 0 | 16 | 64.70 |
| 1.419 | 8 | 0 | 2 | 13 | 65.74 |
| 1.364 | 12 | 1 | 1 | 15 | 68.74 |
| 1.361 | 10 | 0 | 3 | 6 | 68.94 |
| 1.361 | 10 | 3 | 0 | 6 | 68.94 |
| 1.360 | 1 | 2 | 1 | 10 | 68.99 |
| 1.359 | 12 | 2 | 0 | 14 | 69.08 |
| 1.318 | 5 | 1 | 2 | 11 | 71.54 |
| 1.2508 | 17 | 2 | 2 | 0 | 76.03 |
| 1.2344 | 1 | 2 | 1 | 13 | 77.22 |
| 1.2002 | 2 | 1 | 3 | 1 | 79.85 |
| 1.1972 | 3 | 2 | 0 | 17 | 80.09 |
| 1.1956 | 2 | 2 | 2 | 6 | 80.23 |
| 1.1939 | 7 | 1 | 2 | 14 | 80.36 |
| 1.1752 | 2 | 0 | 1 | 20 | 81.91 |
| 1.1629 | 2 | 0 | 0 | 21 | 82.97 |
| 1.1362 | 7 | 1 | 3 | 7 | 85.37 |
| 1.1359 | 1 | 2 | 2 | 9 | 85.40 |
| 1.1182 | 6 | 3 | 1 | 8 | 87.09 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.1165 | 1 | 2 | 1 | 16 | 87.25 |
| 1.1054 | 1 | 0 | 2 | 19 | 88.35 |
| 1.0821 | 3 | 4 | 0 | 1 | 90.77 |
| 1.0804 | 3 | 3 | 0 | 15 | 90.96 |
| 1.0804 | 3 | 0 | 3 | 15 | 90.96 |
| 1.0753 | 2 | 1 | 0 | 22 | 91.51 |
| 1.0665 | 1 | 4 | 0 | 4 | 92.48 |
| 1.0656 | 5 | 2 | 2 | 12 | 92.59 |
| 1.0568 | 2 | 3 | 1 | 11 | 93.59 |
| 1.0545 | 8 | 1 | 1 | 21 | 93.86 |
| 1.0208 | 1 | 0 | 4 | 8 | 97.98 |
| 1.0123 | 1 | 1 | 3 | 13 | 99.10 |

# Cobalt plutonium, $Co_{17}Pu_2$

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with $Ni_{17}Th_2$, from powder data [Ellinger, 1961]. Bouchet et al. [1966] determined positions for $Co_{17}Ho_2$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions for $Co_{17}Ho_2$ were used.

| | |
|---|---|
| 6(g) | 6 cobalt(1) |
| 12(j) | 12 cobalt(2) |
| 12(k) | 12 cobalt(3) |
| 4(f) | 4 cobalt(4) |
| 2(b) | 2 plutonium(1) |
| 2(d) | 2 plutonium(2) |

Lattice constants
a = 8.325 A
c = 8.104 [Ellinger, 1961]

Volume
486.4 $A^3$

Density
(calculated) 10.145 $g/cm^3$

Thermal parameters
Isotropic: cobalt B = 0.6; plutonium B = 0.5.

Scattering factors
$Co^0$ [International Tables, 1962]
$Pu^0$ [International Tables, 1974]

Scale factor (integrated intensities)
$\gamma = 0.399 \times 10^{-3}$

References


Bouchet, G., Laforest, J., Lemaire, R., and Schweizer, J. (1966). C. R. Acad. Sci. Ser. B, 262, 1227.

Ellinger, F. H. (1961). In The Metal Plutonium (Univ. of Chicago Press, Chicago). World Metallurgical Conference, 1957 (edited by Coffinberry, A. S. and Miner, W. N.) p. 288.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 204.

International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 101.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 7.202 | 1 | 1 0 0 | 12.28 |
| 5.381 | 16 | 1 0 1 | 16.46 |
| 4.160 | 19 | 1 1 0 | 21.34 |
| 4.052 | 8 | 0 0 2 | 21.92 |
| 3.604 | 2 | 2 0 0 | 24.68 |
| 3.531 | 6 | 1 0 2 | 25.20 |
| 3.293 | 12 | 2 0 1 | 27.06 |
| 2.903 | 60 | 1 1 2 | 30.78 |
| 2.725 | 2 | 2 1 0 | 32.84 |
| 2.693 | 7 | 2 0 2 | 33.24 |
| 2.583 | 13 | 2 1 1 | 34.70 |
| 2.529 | 11 | 1 0 3 | 35.46 |
| 2.403 | 45 | 3 0 0 | 37.40 |
| 2.261 | 6 | 2 1 2 | 39.84 |
| 2.161 | 25 | 2 0 3 | 41.76 |
| 2.081 | 55 | 2 2 0 | 43.44 |
| 2.067 | 100 | 3 0 2 | 43.76 |
| 2.026 | 25 | 0 0 4 | 44.70 |
| 1.951 | 2 | 1 0 4 | 46.52 |
| 1.942 | 1 | 3 1 1 | 46.74 |
| 1.919 | 14 | 2 1 3 | 47.34 |
| 1.851 | 4 | 2 2 2 | 49.18 |
| 1.793 | 1 | 3 1 2 | 50.88 |
| 1.766 | 3 | 2 0 4 | 51.72 |
| 1.626 | 4 | 2 1 4 | 56.56 |
| 1.621 | 7 | 3 2 1 | 56.76 |
| 1.607 | 3 | 3 1 3 | 57.28 |
| 1.581 | 3 | 1 0 5 | 58.30 |
| 1.573 | 4 | 4 1 0 | 58.64 |
| 1.549 | 10 | 3 0 4 | 59.64 |
| 1.531 | 3 | 3 2 2 | 60.40 |
| 1.499 | 2 | 4 0 3 | 61.84 |
| 1.478 | 1 | 2 0 5 | 62.82 |
| 1.467 | 15 | 4 1 2 | 63.36 |
| 1.452 | 15 | 2 2 4 | 64.10 |
| 1.423 | 1 | 3 1 4 | 65.54 |
| 1.420 | 2 | 5 0 1 | 65.72 |
| 1.411 | 7 | 3 2 3 | 66.20 |
| 1.393 | 5 | 2 1 5 | 67.14 |
| 1.388 | 6 | 3 3 0 | 67.44 |
| 1.359 | 1 | 5 0 2 | 69.08 |
| 1.351 | 1 | 0 0 6 | 69.54 |
| 1.344 | 1 | 4 2 1 | 69.96 |
| 1.313 | 15 | 3 3 2 | 71.86 |
| 1.291 | 1 | 4 2 2 | 73.24 |
| 1.285 | 6 | 1 1 6 | 73.68 |
| 1.281 | 5 | 3 2 4 | 73.90 |
| 1.278 | 3 | 5 1 1 | 74.10 |
| 1.272 | 3 | 5 0 3 | 74.54 |
| 1.259 | 1 | 3 1 5 | 75.44 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.233 | 1 | 5 | 1 | 2 | 77.30 |
| 1.216 | 5 | 4 | 2 | 3 | 78.58 |
| 1.202 | 12 | 6 | 0 | 0 | 79.74 |
| 1.177 | 13 | 3 | 0 | 6 | 81.72 |
| 1.168 | 3 | 5 | 1 | 3 | 82.56 |
| 1.158 | 4 | 3 | 2 | 5 | 83.42 |
| 1.155 | 3 | 5 | 2 | 0 | 83.70 |
| 1.145 | 3 | 3 | 3 | 4 | 84.58 |
| 1.131 | 1 | 4 | 2 | 4 | 85.90 |
| 1.110 | 6 | 5 | 2 | 2 | 87.86 |
| 1.102 | 1 | 2 | 0 | 7 | 88.66 |
| 1.091 | 1 | 5 | 1 | 4 | 89.82 |
| 1.077 | 1 | 5 | 0 | 5 | 91.30 |
| 1.041 | 5 | 4 | 4 | 0 | 95.50 |
| 1.033 | 10 | 6 | 0 | 4 | 96.38 |
| 1.025 | 6 | 4 | 1 | 6 | 97.46 |
| 1.018 | 1 | 6 | 1 | 3 | 98.28 |
| 1.013 | 3 | 0 | 0 | 8 | 99.00 |
| 1.012 | 3 | 5 | 1 | 5 | 99.18 |
| .992 | 1 | 6 | 2 | 1 | 101.84 |
| .984 | 1 | 1 | 1 | 8 | 103.00 |
| .971 | 1 | 6 | 2 | 2 | 105.04 |
| .968 | 7 | 3 | 3 | 6 | 105.48 |
| .962 | 2 | 5 | 3 | 3 | 106.34 |
| .955 | 1 | 7 | 1 | 0 | 107.54 |
| .938 | 4 | 6 | 2 | 3 | 110.48 |
| .933 | 4 | 3 | 0 | 8 | 111.22 |
| .929 | 5 | 7 | 1 | 2 | 111.94 |
| .926 | 5 | 4 | 4 | 4 | 112.64 |
| .918 | 1 | 5 | 3 | 4 | 114.08 |
| .917 | 1 | 5 | 4 | 1 | 114.24 |
| .911 | 5 | 2 | 2 | 8 | 115.50 |
| .908 | 4 | 6 | 3 | 0 | 115.98 |
| .898 | 1 | 6 | 0 | 6 | 118.20 |
| .897 | 1 | 6 | 2 | 4 | 118.44 |
| .894 | 1 | 1 | 0 | 9 | 119.10 |
| .886 | 8 | 6 | 3 | 2 | 120.70 |
| .882 | 2 | 4 | 2 | 7 | 121.64 |
| .878 | 5 | 5 | 2 | 6 | 122.74 |
| .873 | 2 | 5 | 4 | 3 | 123.74 |
| .869 | 2 | 5 | 3 | 5 | 124.78 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 7.210 | 1 | 1 | 0 | 0 | 12.27 |
| 5.387 | 13 | 1 | 0 | 1 | 16.44 |
| 4.163 | 17 | 1 | 1 | 0 | 21.33 |
| 4.052 | 7 | 0 | 0 | 2 | 21.92 |
| 3.605 | 2 | 2 | 0 | 0 | 24.68 |
| 3.532 | 6 | 1 | 0 | 2 | 25.19 |
| 3.294 | 11 | 2 | 0 | 1 | 27.05 |
| 2.903 | 60 | 1 | 1 | 2 | 30.77 |
| 2.725 | 1 | 2 | 1 | 0 | 32.84 |
| 2.693 | 6 | 2 | 0 | 2 | 33.24 |
| 2.583 | 13 | 2 | 1 | 1 | 34.70 |
| 2.530 | 11 | 1 | 0 | 3 | 35.46 |
| 2.403 | 45 | 3 | 0 | 0 | 37.39 |
| 2.261 | 6 | 2 | 1 | 2 | 39.83 |
| 2.162 | 25 | 2 | 0 | 3 | 41.75 |
| 2.081 | 55 | 2 | 2 | 0 | 43.45 |
| 2.067 | 100 | 3 | 0 | 2 | 43.76 |
| 2.026 | 25 | 0 | 0 | 4 | 44.69 |
| 1.950 | 2 | 1 | 0 | 4 | 46.52 |
| 1.941 | 1 | 3 | 1 | 1 | 46.75 |
| 1.918 | 15 | 2 | 1 | 3 | 47.35 |
| 1.851 | 5 | 2 | 2 | 2 | 49.17 |
| 1.793 | 1 | 3 | 1 | 2 | 50.88 |
| 1.766 | 3 | 2 | 0 | 4 | 51.72 |
| 1.654 | 1 | 3 | 2 | 0 | 55.51 |
| 1.626 | 3 | 2 | 1 | 4 | 56.56 |
| 1.621 | 6 | 3 | 2 | 1 | 56.76 |
| 1.607 | 3 | 3 | 1 | 3 | 57.28 |
| 1.581 | 3 | 1 | 0 | 5 | 58.30 |
| 1.573 | 4 | 4 | 1 | 0 | 58.63 |
| 1.549 | 11 | 3 | 0 | 4 | 59.64 |
| 1.531 | 3 | 3 | 2 | 2 | 60.40 |
| 1.499 | 2 | 4 | 0 | 3 | 61.83 |
| 1.478 | 1 | 2 | 0 | 5 | 62.81 |
| 1.467 | 17 | 4 | 1 | 2 | 63.37 |
| 1.452 | 17 | 2 | 2 | 4 | 64.09 |
| 1.423 | 1 | 3 | 1 | 4 | 65.54 |
| 1.420 | 2 | 5 | 0 | 1 | 65.72 |
| 1.411 | 8 | 3 | 2 | 3 | 66.20 |
| 1.393 | 5 | 2 | 1 | 5 | 67.14 |
| 1.388 | 6 | 3 | 3 | 0 | 67.44 |
| 1.358 | 1 | 5 | 0 | 2 | 69.09 |
| 1.351 | 1 | 0 | 0 | 6 | 69.54 |
| 1.344 | 1 | 4 | 2 | 1 | 69.96 |
| 1.313 | 17 | 3 | 3 | 2 | 71.86 |
| 1.291 | 1 | 4 | 2 | 2 | 73.23 |
| 1.285 | 6 | 1 | 1 | 6 | 73.68 |
| 1.281 | 2 | 3 | 2 | 4 | 73.91 |
| 1.279 | 3 | 5 | 1 | 1 | 74.09 |
| 1.272 | 3 | 5 | 0 | 3 | 74.54 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.259 | 2 | 3 | 1 | 5 | 75.44 |
| 1.233 | 1 | 5 | 1 | 2 | 77.29 |
| 1.217 | 5 | 4 | 2 | 3 | 78.57 |
| 1.202 | 14 | 6 | 0 | 0 | 79.74 |
| 1.177 | 16 | 3 | 0 | 6 | 81.72 |
| 1.175 | 1 | 5 | 0 | 4 | 81.95 |
| 1.168 | 4 | 5 | 1 | 3 | 82.55 |
| 1.158 | 4 | 3 | 2 | 5 | 83.43 |
| 1.154 | 2 | 5 | 2 | 0 | 83.71 |
| 1.145 | 3 | 3 | 3 | 4 | 84.58 |
| 1.131 | 1 | 4 | 2 | 4 | 85.89 |
| 1.110 | 7 | 5 | 2 | 2 | 87.86 |
| 1.102 | 2 | 2 | 0 | 7 | 88.67 |
| 1.091 | 1 | 5 | 1 | 4 | 89.82 |
| 1.077 | 2 | 5 | 0 | 5 | 91.29 |
| 1.041 | 6 | 4 | 4 | 0 | 95.50 |
| 1.034 | 12 | 6 | 0 | 4 | 96.37 |
| 1.025 | 8 | 4 | 1 | 6 | 97.47 |
| 1.022 | 1 | 5 | 3 | 1 | 97.86 |
| 1.018 | 1 | 6 | 1 | 3 | 98.30 |
| 1.013 | 3 | 0 | 0 | 8 | 99.00 |
| 1.012 | 3 | 5 | 1 | 5 | 99.18 |
| .998 | 1 | 5 | 3 | 2 | 101.01 |
| .992 | 1 | 6 | 2 | 1 | 101.85 |
| .984 | 1 | 1 | 1 | 8 | 103.00 |
| .971 | 1 | 6 | 2 | 2 | 105.04 |
| .968 | 8 | 3 | 3 | 6 | 105.48 |
| .962 | 3 | 5 | 3 | 3 | 106.34 |
| .955 | 2 | 7 | 1 | 0 | 107.54 |
| .938 | 5 | 6 | 2 | 3 | 110.48 |
| .933 | 5 | 3 | 0 | 8 | 111.22 |
| .929 | 7 | 7 | 1 | 2 | 111.94 |
| .926 | 7 | 4 | 4 | 4 | 112.64 |
| .918 | 1 | 5 | 3 | 4 | 114.07 |
| .917 | 1 | 5 | 4 | 1 | 114.25 |
| .911 | 7 | 2 | 2 | 8 | 115.49 |
| .910 | 1 | 6 | 1 | 5 | 115.69 |
| .908 | 3 | 6 | 3 | 0 | 116.00 |
| .898 | 1 | 6 | 0 | 6 | 118.19 |
| .897 | 1 | 6 | 2 | 4 | 118.44 |
| .894 | 1 | 1 | 0 | 9 | 119.11 |
| .886 | 11 | 6 | 3 | 2 | 120.70 |
| .882 | 2 | 4 | 2 | 7 | 121.65 |
| .878 | 7 | 5 | 2 | 6 | 122.75 |
| .876 | 1 | 7 | 2 | 1 | 123.21 |
| .874 | 3 | 5 | 4 | 3 | 123.73 |
| .869 | 3 | 5 | 3 | 5 | 124.78 |

# Cobalt praseodymium, $Co_2Pr$

Structure
Cubic, Fd3m (227), Z = 8, isostructural with $Cu_2Mg$, from powder data [Harris et al., 1965].

Atom positions
8(a) 8 praseodymium
16(d) 16 cobalt

Lattice constant
a = 7.3063 A
(published value, 7.2911 kX [Harris et al., 1965]).

Volume
390.0 $A^3$

Density
(calculated) 8.814 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$ [Cromer and Mann, 1968]
$Pr^0$ [International Tables, 1974]

Scale factor (integrated intnesities)
$\gamma = 0.575 \times 10^{-3}$

References


Cromer, D.T. and Mann, J.B. (1968). Acta Crystallogr. A24, 321.

Harris, I. R., Mansey, R. C., and Raynor, G. V. (1965). J. Less-Common Metals 9, 270.

International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 100.


Calculated Pattern (Peak heights)

| d(A) | I | hkl | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 4.215 | 10 | 1 1 1 | 21.06 |
| 2.583 | 65 | 2 2 0 | 34.70 |
| 2.203 | 100 | 3 1 1 | 40.94 |
| 2.109 | 15 | 2 2 2 | 42.84 |
| 1.676 | 1 | 3 3 1 | 54.72 |
| 1.4913 | 15 | 4 2 2 | 62.20 |
| 1.4060 | 25 | 5 1 1+ | 66.44 |
| 1.2917 | 15 | 4 4 0 | 73.22 |
| 1.2350 | 1 | 5 3 1 | 77.18 |
| 1.1552 | 5 | 6 2 0 | 83.64 |
| 1.1141 | 5 | 5 3 3 | 87.48 |
| 1.1015 | 5 | 6 2 2 | 88.74 |
| 1.0231 | 1 | 7 1 1+ | 97.68 |
| .9763 | 5 | 6 4 2 | 104.18 |
| .9512 | 10 | 7 3 1+ | 108.16 |
| .9133 | 1 | 8 0 0 | 115.00 |
| .8610 | 5 | 8 2 2+ | 126.92 |
| .8437 | 10 | 7 5 1+ | 131.86 |
| .8381 | 1 | 6 6 2 | 133.60 |
| .8020 | 1 | 7 5 3+ | 147.68 |

Calculated Pattern (Integrated)

| d(A) | I | hkl | 2θ(°) λ = 1.540598A |
|---|---|---|---|
| 4.218 | 10 | 1 1 1 | 21.04 |
| 2.583 | 60 | 2 2 0 | 34.70 |
| 2.203 | 100 | 3 1 1 | 40.93 |
| 2.109 | 15 | 2 2 2 | 42.84 |
| 1.676 | 1 | 3 3 1 | 54.72 |
| 1.4914 | 20 | 4 2 2 | 62.20 |
| 1.4061 | 20 | 5 1 1 | 66.44 |
| 1.4061 | 5 | 3 3 3 | 66.44 |
| 1.2916 | 20 | 4 4 0 | 73.22 |
| 1.2350 | 1 | 5 3 1 | 77.18 |
| 1.1552 | 5 | 6 2 0 | 83.64 |
| 1.1142 | 10 | 5 3 3 | 87.47 |
| 1.1015 | 5 | 6 2 2 | 88.75 |
| .9763 | 10 | 6 4 2 | 104.18 |
| .9512 | 10 | 7 3 1 | 108.16 |
| .9512 | 5 | 5 5 3 | 108.16 |
| .9133 | 5 | 8 0 0 | 115.01 |
| .8611 | 1 | 6 6 0 | 126.91 |
| .8611 | 5 | 8 2 2 | 126.91 |
| .8437 | 10 | 7 5 1 | 131.86 |
| .8437 | 1 | 5 5 5 | 131.86 |
| .8381 | 5 | 6 6 2 | 133.59 |
| .8020 | 1 | 7 5 3 | 147.69 |
| .8020 | 1 | 9 1 1 | 147.69 |

# Cobalt rhodium sulfide, $Co_8RhS_8$

Structure
Cubic, Fm3m (225), Z = 4, π phase, isostructural with $Co_9S_8$, from powder data [Knop, 1962].

Atom positions [Pearson, 1967]
32(f) 32 cobalt 8(c) 8 sulfur
4(b) 4 rhodium 24(e) 24 sulfur

Lattice constant
a = 9.978(2) Å
(published value, a = 9.977(2) Å, [Knop, 1962])

Volume
993.4 $Å^3$

Density
(calculated) 5.555 $g/cm^3$

Thermal parameters
Isotropic: cobalt, B = 0.5; rhodium, B = 0.4; sulfur, B = 0.7

Scattering factors
$Co^0$, $Rh^0$, $S^0$ [International tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.413 \times 10^{-3}$

References


International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England). pp. 202, 204, 210.

Knop, D. (1962). Chem. Ind. London, April 21, p. 739.

Pearson, W. B. (1967). Handbook of Lattice Spacings and Structures of Metals and Alloys, v.2, (Pergamon Press, N.Y.), pp. 204, 807.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
|---|---|---|---|---|---|
| 5.757 | 7 | 1 | 1 | 1 | 15.38 |
| 4.985 | 12 | 2 | 0 | 0 | 17.78 |
| 3.526 | 12 | 2 | 2 | 0 | 25.24 |
| 3.008 | 100 | 3 | 1 | 1 | 29.68 |
| 2.881 | 10 | 2 | 2 | 2 | 31.02 |
| 2.494 | 3 | 4 | 0 | 0 | 35.98 |
| 2.288 | 5 | 3 | 3 | 1 | 39.34 |
| 2.231 | 7 | 4 | 2 | 0 | 40.40 |
| 2.037 | 4 | 4 | 2 | 2 | 44.44 |
| 1.920 | 30 | 5 | 1 | 1+ | 47.30 |
| 1.763 | 75 | 4 | 4 | 0 | 51.80 |
| 1.686 | 1 | 5 | 3 | 1 | 54.36 |
| 1.663 | 2 | 4 | 4 | 2+ | 55.18 |
| 1.577 | 2 | 6 | 2 | 0 | 58.46 |
| 1.522 | 9 | 5 | 3 | 3 | 60.82 |
| 1.504 | 2 | 6 | 2 | 2 | 61.60 |
| 1.3334 | 2 | 6 | 4 | 2 | 70.58 |
| 1.2990 | 14 | 7 | 3 | 1+ | 72.74 |
| 1.2473 | 9 | 8 | 0 | 0 | 76.28 |
| 1.2190 | 1 | 7 | 3 | 3 | 78.38 |
| 1.2100 | 1 | 6 | 4 | 4+ | 79.08 |
| 1.1760 | 1 | 8 | 2 | 2+ | 81.84 |
| 1.1521 | 7 | 7 | 5 | 1+ | 83.92 |
| 1.1446 | 1 | 6 | 6 | 2 | 84.60 |
| 1.0886 | 1 | 8 | 4 | 2 | 90.08 |
| 1.0460 | 5 | 9 | 3 | 1 | 94.86 |
| 1.0183 | 18 | 8 | 4 | 4 | 98.30 |
| .9785 | 1 | 8 | 6 | 2+ | 103.86 |
| .9646 | 6 | 9 | 5 | 1+ | 105.98 |
| .9601 | 1 | 10 | 2 | 2+ | 106.70 |
| .9264 | 1 | 10 | 4 | 0+ | 112.50 |
| .8997 | 3 | 11 | 1 | 1+ | 117.78 |
| .8819 | 7 | 8 | 8 | 0 | 121.72 |
| .8463 | 4 | 9 | 7 | 3+ | 131.06 |
| .8433 | 1 | 10 | 6 | 2 | 131.96 |
| .8093 | 1 | 10 | 6 | 4+ | 144.28 |
| .8015 | 6 | 9 | 7 | 5+ | 147.94 |
| .7888 | 14 | 12 | 4 | 0 | 155.12 |
| .7792 | 1 | 8 | 8 | 6+ | 162.70 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 5.761 | 6 | 1 | 1 | 1 | 15.37 |
| 4.989 | 11 | 2 | 0 | 0 | 17.76 |
| 3.528 | 11 | 2 | 2 | 0 | 25.22 |
| 3.008 | 100 | 3 | 1 | 1 | 29.67 |
| 2.880 | 10 | 2 | 2 | 2 | 31.02 |
| 2.494 | 3 | 4 | 0 | 0 | 35.97 |
| 2.289 | 5 | 3 | 3 | 1 | 39.33 |
| 2.231 | 7 | 4 | 2 | 0 | 40.39 |
| 2.037 | 4 | 4 | 2 | 2 | 44.44 |
| 1.920 | 30 | 5 | 1 | 1 | 47.30 |
| 1.920 | 8 | 3 | 3 | 3 | 47.30 |
| 1.764 | 85 | 4 | 4 | 0 | 51.79 |
| 1.687 | 1 | 5 | 3 | 1 | 54.35 |
| 1.663 | 1 | 6 | 0 | 0 | 55.19 |
| 1.663 | 2 | 4 | 4 | 2 | 55.19 |
| 1.578 | 2 | 6 | 2 | 0 | 58.45 |
| 1.522 | 11 | 5 | 3 | 3 | 60.83 |
| 1.504 | 2 | 6 | 2 | 2 | 61.61 |
| 1.4402 | 1 | 4 | 4 | 4 | 64.67 |
| 1.3972 | 1 | 7 | 1 | 1 | 66.91 |
| 1.3837 | 1 | 6 | 4 | 0 | 67.66 |
| 1.3334 | 2 | 6 | 4 | 2 | 70.58 |
| 1.2990 | 11 | 7 | 3 | 1 | 72.74 |
| 1.2990 | 7 | 5 | 5 | 3 | 72.74 |
| 1.2472 | 11 | 8 | 0 | 0 | 76.28 |
| 1.2190 | 1 | 7 | 3 | 3 | 78.38 |
| 1.2100 | 1 | 6 | 4 | 4 | 79.08 |
| 1.1522 | 8 | 7 | 5 | 1 | 83.91 |
| 1.1522 | 2 | 5 | 5 | 5 | 83.91 |
| 1.1446 | 1 | 6 | 6 | 2 | 84.60 |
| 1.0887 | 1 | 8 | 4 | 2 | 90.07 |
| 1.0460 | 7 | 9 | 3 | 1 | 94.86 |
| 1.0184 | 25 | 8 | 4 | 4 | 98.30 |
| .9784 | 1 | 8 | 6 | 2 | 103.87 |
| .9646 | 6 | 9 | 5 | 1 | 105.99 |
| .9646 | 2 | 7 | 7 | 3 | 105.99 |
| .9264 | 1 | 10 | 4 | 0 | 112.50 |
| .9109 | 1 | 10 | 4 | 2 | 115.49 |
| .8997 | 2 | 11 | 1 | 1 | 117.78 |
| .8997 | 2 | 7 | 7 | 5 | 117.78 |
| .8819 | 11 | 8 | 8 | 0 | 121.72 |
| .8718 | 1 | 11 | 3 | 1 | 124.16 |
| .8463 | 2 | 11 | 3 | 3 | 131.06 |
| .8463 | 5 | 9 | 7 | 3 | 131.06 |
| .8433 | 1 | 10 | 6 | 2 | 131.97 |
| .8093 | 2 | 10 | 6 | 4 | 144.27 |
| .8015 | 7 | 11 | 5 | 3 | 147.94 |
| .8015 | 9 | 9 | 7 | 5 | 147.94 |
| .7888 | 45 | 12 | 4 | 0 | 155.11 |
| .7792 | 2 | 8 | 8 | 6 | 162.71 |
| .7792 | 2 | 12 | 4 | 2 | 162.71 |

# Cobalt ruthenium sulfide, $Co_8RuS_8$

Structure
Cubic, Fm3m (225), Z = 4, π phase, isostructural with $Co_9S_8$, from powder data [Knop, 1962].

Atom positions [Pearson, 1967].

| | | | |
|---|---|---|---|
| 32(f) | 32 cobalt | 8(c) | 8 sulfur |
| 4(b) | 4 ruthenium | 24(e) | 24 sulfur |

Lattice constant [Knop, 1962]
a = 9.945(2)A
(published value, a = 9.944(2) Å)

Volume
983.6 $Å^3$

Density
(calculated) 5.599 $g/cm^3$

Thermal parameters
Isotropic: cobalt, B = 0.5; ruthenium, B = 0.4; sulfur, B = 0.7

Scattering factors
$Co^0$, $Ru^0$, $S^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.409 \times 10^{-3}$

References


International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, England) pp. 202, 204, 210.

Knop, O. (1962). Chem. Ind. London, April 21, p. 739.

Pearson, W.B. (1967). Handbook of Lattice Spacings and Structures of Metals and Alloys, V.2, (Pergamon Press, N.Y.). pp. 204, 808.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 5.734 | 8 | 1 1 1 | 15.44 |
| 4.968 | 12 | 2 0 0 | 17.84 |
| 3.515 | 11 | 2 2 0 | 25.32 |
| 2.998 | 100 | 3 1 1 | 29.78 |
| 2.870 | 10 | 2 2 2 | 31.14 |
| 2.486 | 3 | 4 0 0 | 36.10 |
| 2.282 | 5 | 3 3 1 | 39.46 |
| 2.223 | 6 | 4 2 0 | 40.54 |
| 2.030 | 4 | 4 2 2 | 44.60 |
| 1.9141 | 30 | 5 1 1+ | 47.46 |
| 1.7578 | 75 | 4 4 0 | 51.98 |
| 1.6812 | 1 | 5 3 1 | 54.54 |
| 1.6577 | 2 | 4 4 2+ | 55.38 |
| 1.5726 | 2 | 6 2 0 | 58.66 |
| 1.5164 | 9 | 5 3 3 | 61.06 |
| 1.4991 | 2 | 6 2 2 | 61.84 |
| 1.3291 | 2 | 6 4 2 | 70.84 |
| 1.2947 | 14 | 7 3 1+ | 73.02 |
| 1.2431 | 9 | 8 0 0 | 76.58 |
| 1.2149 | 1 | 7 3 3 | 78.70 |
| 1.2059 | 1 | 6 4 4+ | 79.40 |
| 1.1720 | 1 | 8 2 2+ | 82.18 |
| 1.1483 | 7 | 7 5 1+ | 84.26 |
| 1.1408 | 1 | 6 6 2 | 84.94 |
| 1.0850 | 1 | 8 4 2 | 90.46 |
| 1.0425 | 5 | 9 3 1 | 95.28 |
| 1.0150 | 19 | 8 4 4 | 98.74 |
| .9751 | 1 | 8 6 2+ | 104.36 |
| .9614 | 6 | 9 5 1+ | 106.50 |
| .9570 | 1 | 10 2 2+ | 107.20 |
| .9233 | 1 | 10 4 0+ | 113.08 |
| .8967 | 3 | 11 1 1+ | 118.42 |
| .8790 | 7 | 8 8 0 | 122.40 |
| .8435 | 4 | 9 7 3+ | 131.90 |
| .8405 | 1 | 10 6 2 | 132.82 |
| .8067 | 1 | 10 6 4+ | 145.46 |
| .7988 | 6 | 9 7 5+ | 149.30 |
| .7862 | 14 | 12 4 0 | 156.90 |

Cobalt ruthenium sulfide, $Co_8RuS_8$ - (continued)

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 5.742 | 7 | 1 | 1 | 1 | 15.42 |
| 4.973 | 10 | 2 | 0 | 0 | 17.82 |
| 3.516 | 11 | 2 | 2 | 0 | 25.31 |
| 2.999 | 100 | 3 | 1 | 1 | 29.77 |
| 2.871 | 10 | 2 | 2 | 2 | 31.13 |
| 2.486 | 3 | 4 | 0 | 0 | 36.10 |
| 2.282 | 6 | 3 | 3 | 1 | 39.46 |
| 2.224 | 7 | 4 | 2 | 0 | 40.53 |
| 2.030 | 4 | 4 | 2 | 2 | 44.60 |
| 1.9139 | 30 | 5 | 1 | 1 | 47.47 |
| 1.9139 | 8 | 3 | 3 | 3 | 47.47 |
| 1.7580 | 85 | 4 | 4 | 0 | 51.97 |
| 1.6810 | 1 | 5 | 3 | 1 | 54.55 |
| 1.6575 | 1 | 6 | 0 | 0 | 55.39 |
| 1.6575 | 2 | 4 | 4 | 2 | 55.39 |
| 1.5724 | 2 | 6 | 2 | 0 | 58.66 |
| 1.5166 | 11 | 5 | 3 | 3 | 61.05 |
| 1.4993 | 2 | 6 | 2 | 2 | 61.83 |
| 1.4354 | 1 | 4 | 4 | 4 | 64.91 |
| 1.3926 | 1 | 7 | 1 | 1 | 67.17 |
| 1.3290 | 2 | 6 | 4 | 2 | 70.85 |
| 1.2947 | 11 | 7 | 3 | 1 | 73.02 |
| 1.2947 | 7 | 5 | 5 | 3 | 73.02 |
| 1.2431 | 12 | 8 | 0 | 0 | 76.58 |
| 1.2150 | 1 | 7 | 3 | 3 | 78.69 |
| 1.2060 | 1 | 6 | 4 | 4 | 79.39 |
| 1.1483 | 8 | 7 | 5 | 1 | 84.26 |
| 1.1483 | 2 | 5 | 5 | 5 | 84.26 |
| 1.1408 | 1 | 6 | 6 | 2 | 84.95 |
| 1.0851 | 1 | 8 | 4 | 2 | 90.45 |
| 1.0425 | 6 | 9 | 3 | 1 | 95.27 |
| 1.0150 | 25 | 8 | 4 | 4 | 98.74 |
| .9752 | 1 | 8 | 6 | 2 | 104.35 |
| .9614 | 2 | 7 | 7 | 3 | 106.49 |
| .9614 | 6 | 9 | 5 | 1 | 106.49 |
| .9234 | 1 | 10 | 4 | 0 | 113.07 |
| .9079 | 1 | 10 | 4 | 2 | 116.10 |
| .8967 | 2 | 11 | 1 | 1 | 118.42 |
| .8967 | 2 | 7 | 7 | 5 | 118.42 |
| .8790 | 11 | 8 | 8 | 0 | 122.40 |
| .8689 | 1 | 11 | 3 | 1 | 124.88 |
| .8435 | 6 | 9 | 7 | 3 | 131.90 |
| .8435 | 2 | 11 | 3 | 3 | 131.90 |
| .8405 | 1 | 10 | 6 | 2 | 132.83 |
| .8066 | 2 | 10 | 6 | 4 | 145.47 |
| .7988 | 9 | 9 | 7 | 5 | 149.30 |
| .7988 | 7 | 11 | 5 | 3 | 149.30 |
| .7862 | 47 | 12 | 4 | 0 | 156.90 |

# Cobalt tantalum silicide, $Co_{16}Ta_6Si_7$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions of $Co_{16}Nb_6Si_7$ were preferred.

| | |
|---|---|
| 32(f) | 32 cobalt (1) |
| 32(f) | 32 cobalt (2) |
| 4(b) | 4 silicon (1) |
| 24(d) | 24 silicon (2) |
| 24(e) | 24 tantalum |

Lattice constant
a = 11.199 Å
(published value, 11.198 Å [Spiegel et al., 1963]).

Volume
1404.6 $Å^3$

Density
(calculated) 10.523 $g/cm^3$

Thermal parameters
Isotropic: cobalt B = 1.0; silicon B = 1.0; tantalum B = 0.8.

Scattering factors
$Co^0$, $Si^0$, $Ta^0$ [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.361 \times 10^{-3}$

References


International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), pp. 202, 204, 212.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 6.458 | 25 | 1 1 1 | 13.70 |
| 5.597 | 8 | 2 0 0 | 15.82 |
| 3.959 | 1 | 2 2 0 | 22.44 |
| 3.232 | 40 | 2 2 2 | 27.58 |
| 2.800 | 2 | 4 0 0 | 31.94 |
| 2.569 | 30 | 3 3 1 | 34.90 |
| 2.504 | 6 | 4 2 0 | 35.84 |
| 2.286 | 35 | 4 2 2 | 39.38 |
| 2.155 | 100 | 5 1 1+ | 41.88 |
| 1.980 | 45 | 4 4 0 | 45.80 |
| 1.893 | 3 | 5 3 1 | 48.02 |
| 1.866 | 25 | 6 0 0 | 48.76 |
| 1.568 | 12 | 5 5 1 | 58.84 |
| 1.553 | 4 | 6 4 0 | 59.48 |
| 1.458 | 8 | 7 3 1+ | 63.78 |
| 1.400 | 2 | 8 0 0 | 66.78 |
| 1.368 | 9 | 7 3 3 | 68.52 |
| 1.358 | 2 | 6 4 4+ | 69.10 |
| 1.320 | 20 | 8 2 2+ | 71.42 |
| 1.293 | 11 | 5 5 5+ | 73.12 |
| 1.229 | 4 | 7 5 3 | 77.60 |
| 1.222 | 9 | 8 4 2 | 78.16 |
| 1.125 | 14 | 9 3 3+ | 86.38 |
| 1.120 | 2 | 10 0 0 | 86.92 |
| 1.098 | 3 | 10 2 0+ | 89.08 |
| 1.083 | 6 | 7 7 3+ | 90.72 |
| 1.078 | 3 | 6 6 6 | 91.26 |
| 1.040 | 3 | 10 4 0 | 95.60 |
| 1.010 | 2 | 11 1 1 | 99.44 |
| .9785 | 2 | 9 7 1+ | 103.86 |
| .9747 | 6 | 8 8 2+ | 104.42 |
| .9604 | 2 | 10 6 0 | 106.66 |
| .9499 | 1 | 9 7 3 | 108.38 |
| .9465 | 2 | 10 6 2 | 108.94 |
| .9332 | 4 | 8 8 4+ | 111.26 |
| .9236 | 4 | 11 5 1+ | 113.02 |
| .9083 | 5 | 10 6 4+ | 116.00 |
| .8995 | 1 | 11 5 3+ | 117.82 |
| .8854 | 2 | 12 4 0 | 120.92 |
| .8745 | 2 | 10 8 0+ | 123.50 |
| .8640 | 1 | 10 8 2 | 126.14 |
| .8564 | 8 | 11 5 5+ | 128.18 |
| .8542 | 5 | 10 6 6 | 128.78 |
| .8371 | 8 | 13 3 1+ | 133.92 |
| .8349 | 6 | 12 6 0 | 134.62 |
| .8256 | 1 | 12 6 2 | 137.82 |
| .8190 | 3 | 13 3 3+ | 140.30 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 6.466 | 40 | 1 | 1 | 1 | 13.68 |
| 5.599 | 12 | 2 | 0 | 0 | 15.81 |
| 3.959 | 2 | 2 | 2 | 0 | 22.44 |
| 3.377 | 1 | 3 | 1 | 1 | 26.37 |
| 3.233 | 70 | 2 | 2 | 2 | 27.57 |
| 2.800 | 4 | 4 | 0 | 0 | 31.94 |
| 2.569 | 50 | 3 | 3 | 1 | 34.89 |
| 2.504 | 10 | 4 | 2 | 0 | 35.83 |
| 2.286 | 60 | 4 | 2 | 2 | 39.38 |
| 2.155 | 100 | 5 | 1 | 1 | 41.88 |
| 2.155 | 85 | 3 | 3 | 3 | 41.88 |
| 1.980 | 85 | 4 | 4 | 0 | 45.80 |
| 1.893 | 6 | 5 | 3 | 1 | 48.02 |
| 1.866 | 40 | 6 | 0 | 0 | 48.75 |
| 1.866 | 6 | 4 | 4 | 2 | 48.75 |
| 1.616 | 1 | 4 | 4 | 4 | 56.92 |
| 1.568 | 25 | 5 | 5 | 1 | 58.84 |
| 1.553 | 8 | 6 | 4 | 0 | 59.47 |
| 1.458 | 11 | 7 | 3 | 1 | 63.79 |
| 1.458 | 6 | 5 | 5 | 3 | 63.79 |
| 1.400 | 5 | 8 | 0 | 0 | 66.77 |
| 1.368 | 19 | 7 | 3 | 3 | 68.53 |
| 1.358 | 3 | 6 | 4 | 4 | 69.11 |
| 1.320 | 19 | 6 | 6 | 0 | 71.41 |
| 1.320 | 25 | 8 | 2 | 2 | 71.41 |
| 1.293 | 10 | 7 | 5 | 1 | 73.12 |
| 1.293 | 13 | 5 | 5 | 5 | 73.12 |
| 1.229 | 8 | 7 | 5 | 3 | 77.61 |
| 1.222 | 18 | 8 | 4 | 2 | 78.16 |
| 1.194 | 1 | 6 | 6 | 4 | 80.37 |
| 1.143 | 1 | 8 | 4 | 4 | 84.74 |
| 1.126 | 25 | 9 | 3 | 3 | 86.37 |
| 1.126 | 2 | 7 | 7 | 1 | 86.37 |
| 1.126 | 2 | 7 | 5 | 5 | 86.37 |
| 1.120 | 3 | 10 | 0 | 0 | 86.92 |
| 1.098 | 3 | 8 | 6 | 2 | 89.09 |
| 1.098 | 3 | 10 | 2 | 0 | 89.09 |
| 1.083 | 7 | 7 | 7 | 3 | 90.71 |
| 1.083 | 6 | 9 | 5 | 1 | 90.71 |
| 1.078 | 7 | 6 | 6 | 6 | 91.26 |
| 1.040 | 6 | 10 | 4 | 0 | 95.60 |
| 1.010 | 5 | 11 | 1 | 1 | 99.43 |
| .9899 | 1 | 8 | 8 | 0 | 102.19 |
| .9785 | 3 | 9 | 7 | 1 | 103.86 |
| .9785 | 1 | 9 | 5 | 5 | 103.86 |
| .9747 | 12 | 8 | 8 | 2 | 104.42 |
| .9747 | 2 | 10 | 4 | 4 | 104.42 |
| .9603 | 5 | 10 | 6 | 0 | 106.67 |
| .9499 | 2 | 9 | 7 | 3 | 108.38 |
| .9465 | 6 | 10 | 6 | 2 | 108.95 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .9332 | 9 | 8 | 8 | 4 | 111.26 |
| .9332 | 2 | 12 | 0 | 0 | 111.26 |
| .9237 | 9 | 11 | 5 | 1 | 113.01 |
| .9237 | 2 | 7 | 7 | 7 | 113.01 |
| .9206 | 1 | 12 | 2 | 0 | 113.60 |
| .9084 | 4 | 12 | 2 | 2 | 115.99 |
| .9084 | 8 | 10 | 6 | 4 | 115.99 |
| .8995 | 2 | 11 | 5 | 3 | 117.82 |
| .8854 | 5 | 12 | 4 | 0 | 120.93 |
| .8745 | 2 | 12 | 4 | 2 | 123.49 |
| .8745 | 2 | 10 | 8 | 0 | 123.49 |
| .8745 | 2 | 8 | 8 | 6 | 123.49 |
| .8640 | 3 | 10 | 8 | 2 | 126.13 |
| .8564 | 15 | 11 | 5 | 5 | 128.17 |
| .8564 | 3 | 11 | 7 | 1 | 128.17 |
| .8564 | 5 | 9 | 9 | 3 | 128.17 |
| .8539 | 7 | 10 | 6 | 6 | 128.87 |
| .8371 | 16 | 13 | 3 | 1 | 133.93 |
| .8371 | 5 | 11 | 7 | 3 | 133.93 |
| .8371 | 6 | 9 | 7 | 7 | 133.93 |
| .8347 | 9 | 12 | 6 | 0 | 134.68 |
| .8256 | 4 | 12 | 6 | 2 | 137.82 |
| .8190 | 8 | 13 | 3 | 3 | 140.30 |
| .8190 | 5 | 9 | 9 | 5 | 140.30 |
| .8082 | 2 | 8 | 8 | 8 | 144.76 |

# Cobalt titanium silicide, $Co_{16}Ti_6Si_7$

Structure
Cubic, Fm3m (225), Z = 4, isostructural with $Cu_{16}Mg_6Si_7$, from powder data [Spiegel et al., 1963]. Kuz'ma et al. [1964] determined positions for $Co_{16}Nb_6Si_7$, a similar isostructural compound.

Atom positions
From considerations of atomic size, the positions for $Co_{16}Nb_6Si_7$ were preferred.

| | |
|---|---|
| 32(f) | 32 cobalt (1) |
| 32(f) | 32 cobalt (2) |
| 4(b) | 4 silicon (1) |
| 24(d) | 24 silicon (2) |
| 24(e) | 24 titanium |

Lattice constant
a = 11.202 Å
(published value, 11.201 Å [Spiegel et al., 1963])

Volume
1405.7 $Å^3$

Density
(calculated) 6.743 $g/cm^3$

Thermal parameters
Isotropic: overall B = 1.0

Scattering factors
$Co^0$, $Si^0$, $Ti^0$ [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.215 \times 10^{-3}$

References


International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204.

Kuz'ma, Yu. B., Gladyshevs'kii, E. I., and Byk, D. S. (1964). J. Struct. Chem. (USSR) 5, 518.

Spiegel, F. X., Bardos, D., and Beck, P. A. (1963). Trans. AIME 227, 575.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 6.458 | 6 | 1 1 1 | 13.70 |
| 5.597 | 30 | 2 0 0 | 15.82 |
| 3.959 | 3 | 2 2 0 | 22.44 |
| 3.234 | 2 | 2 2 2 | 27.56 |
| 2.800 | 20 | 4 0 0 | 31.94 |
| 2.570 | 4 | 3 3 1 | 34.88 |
| 2.505 | 7 | 4 2 0 | 35.82 |
| 2.286 | 20 | 4 2 2 | 39.38 |
| 2.155 | 90 | 5 1 1+ | 41.88 |
| 1.980 | 100 | 4 4 0 | 45.78 |
| 1.893 | 35 | 5 3 1 | 48.02 |
| 1.867 | 25 | 6 0 0 | 48.74 |
| 1.771 | 7 | 6 2 0 | 51.56 |
| 1.708 | 15 | 5 3 3 | 53.60 |
| 1.689 | 8 | 6 2 2 | 54.28 |
| 1.617 | 3 | 4 4 4 | 56.90 |
| 1.569 | 2 | 7 1 1+ | 58.82 |
| 1.497 | 1 | 6 4 2 | 61.94 |
| 1.459 | 2 | 7 3 1+ | 63.76 |
| 1.400 | 4 | 8 0 0 | 66.76 |
| 1.369 | 1 | 7 3 3 | 68.50 |
| 1.359 | 1 | 6 4 4+ | 69.08 |
| 1.320 | 14 | 6 6 0+ | 71.40 |
| 1.293 | 9 | 7 5 1+ | 73.10 |
| 1.230 | 11 | 7 5 3+ | 77.58 |
| 1.222 | 4 | 8 4 2 | 78.14 |
| 1.174 | 6 | 9 3 1 | 81.98 |
| 1.143 | 8 | 8 4 4 | 84.72 |
| 1.126 | 17 | 9 3 3 | 86.34 |
| 1.120 | 3 | 8 6 0 | 86.88 |
| 1.083 | 2 | 9 5 1+ | 90.68 |
| 1.078 | 5 | 6 6 6 | 91.22 |
| 1.040 | 1 | 10 4 0+ | 95.56 |
| 1.010 | 2 | 11 1 1+ | 99.40 |
| .9901 | 4 | 8 8 0 | 102.16 |
| .9787 | 6 | 9 7 1+ | 103.82 |
| .9750 | 2 | 8 8 2 | 104.38 |
| .9606 | 1 | 8 6 6 | 106.62 |
| .9501 | 2 | 9 7 3+ | 108.34 |
| .9468 | 4 | 10 6 2 | 108.90 |
| .9335 | 3 | 8 8 4 | 111.22 |
| .9208 | 1 | 12 2 0 | 113.56 |
| .9086 | 1 | 10 6 4 | 115.94 |
| .8856 | 3 | 12 4 0 | 120.88 |
| .8567 | 5 | 11 5 5+ | 128.10 |
| .8373 | 8 | 13 3 1+ | 133.86 |
| .8351 | 7 | 12 6 0 | 134.56 |
| .8258 | 2 | 12 6 2 | 137.74 |
| .8192 | 2 | 9 9 5 | 140.22 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | h | k | ℓ | 2θ(°) λ = 1.540598Å |
| 6.467 | 5 | 1 | 1 | 1 | 13.68 |
| 5.601 | 25 | 2 | 0 | 0 | 15.81 |
| 3.961 | 3 | 2 | 2 | 0 | 22.43 |
| 3.234 | 2 | 2 | 2 | 2 | 27.56 |
| 2.800 | 19 | 4 | 0 | 0 | 31.93 |
| 2.570 | 4 | 3 | 3 | 1 | 34.88 |
| 2.505 | 7 | 4 | 2 | 0 | 35.82 |
| 2.287 | 19 | 4 | 2 | 2 | 39.37 |
| 2.156 | 45 | 5 | 1 | 1 | 41.87 |
| 2.156 | 40 | 3 | 3 | 3 | 41.87 |
| 1.980 | 100 | 4 | 4 | 0 | 45.78 |
| 1.893 | 35 | 5 | 3 | 1 | 48.01 |
| 1.867 | 20 | 6 | 0 | 0 | 48.73 |
| 1.867 | 3 | 4 | 4 | 2 | 48.73 |
| 1.771 | 7 | 6 | 2 | 0 | 51.56 |
| 1.708 | 15 | 5 | 3 | 3 | 53.61 |
| 1.689 | 8 | 6 | 2 | 2 | 54.28 |
| 1.617 | 4 | 4 | 4 | 4 | 56.90 |
| 1.569 | 2 | 7 | 1 | 1 | 58.82 |
| 1.497 | 1 | 6 | 4 | 2 | 61.94 |
| 1.458 | 1 | 7 | 3 | 1 | 63.77 |
| 1.458 | 1 | 5 | 5 | 3 | 63.77 |
| 1.400 | 4 | 8 | 0 | 0 | 66.75 |
| 1.369 | 2 | 7 | 3 | 3 | 68.51 |
| 1.358 | 1 | 6 | 4 | 4 | 69.09 |
| 1.320 | 10 | 6 | 6 | 0 | 71.39 |
| 1.320 | 5 | 8 | 2 | 2 | 71.39 |
| 1.293 | 6 | 7 | 5 | 1 | 73.10 |
| 1.293 | 4 | 5 | 5 | 5 | 73.10 |
| 1.252 | 1 | 8 | 4 | 0 | 75.91 |
| 1.230 | 3 | 9 | 1 | 1 | 77.58 |
| 1.230 | 9 | 7 | 5 | 3 | 77.58 |
| 1.222 | 5 | 8 | 4 | 2 | 78.14 |
| 1.194 | 1 | 6 | 6 | 4 | 80.34 |
| 1.174 | 7 | 9 | 3 | 1 | 81.99 |
| 1.143 | 9 | 8 | 4 | 4 | 84.71 |
| 1.126 | 19 | 9 | 3 | 3 | 86.35 |
| 1.126 | 1 | 7 | 7 | 1 | 86.35 |
| 1.120 | 2 | 8 | 6 | 0 | 86.89 |
| 1.098 | 1 | 10 | 2 | 0 | 89.06 |
| 1.083 | 1 | 9 | 5 | 1 | 90.68 |
| 1.078 | 5 | 6 | 6 | 6 | 91.22 |
| 1.010 | 2 | 11 | 1 | 1 | 99.39 |
| .9901 | 5 | 8 | 8 | 0 | 102.15 |
| .9787 | 4 | 9 | 7 | 1 | 103.82 |
| .9787 | 3 | 11 | 3 | 1 | 103.82 |
| .9787 | 1 | 9 | 5 | 5 | 103.82 |
| .9750 | 2 | 8 | 8 | 2 | 104.38 |
| .9606 | 1 | 8 | 6 | 6 | 106.63 |
| .9501 | 1 | 9 | 7 | 3 | 108.33 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | h | k | ℓ | 2θ(°) λ = 1.540598Å |
| .9501 | 1 | 11 | 3 | 3 | 108.33 |
| .9467 | 5 | 10 | 6 | 2 | 108.90 |
| .9335 | 4 | 8 | 8 | 4 | 111.21 |
| .9208 | 1 | 12 | 2 | 0 | 113.56 |
| .9086 | 1 | 10 | 6 | 4 | 115.94 |
| .8856 | 4 | 12 | 4 | 0 | 120.87 |
| .8747 | 1 | 10 | 8 | 0 | 123.43 |
| .8643 | 1 | 10 | 8 | 2 | 126.07 |
| .8566 | 3 | 11 | 5 | 5 | 128.11 |
| .8566 | 1 | 11 | 7 | 1 | 128.11 |
| .8566 | 3 | 9 | 9 | 3 | 128.11 |
| .8373 | 7 | 13 | 3 | 1 | 133.85 |
| .8373 | 4 | 11 | 7 | 3 | 133.85 |
| .8373 | 3 | 9 | 7 | 7 | 133.85 |
| .8349 | 6 | 12 | 6 | 0 | 134.61 |
| .8258 | 4 | 12 | 6 | 2 | 137.74 |
| .8192 | 5 | 9 | 9 | 5 | 140.22 |
| .8084 | 1 | 8 | 8 | 8 | 144.66 |

# Diazepam, $C_{16}H_{13}ClN_2O$

Synonym
7-chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one

Structure
Monoclinic, $P2_1/a$ (14), Z = 4. The structure was determined by Camerman and Camerman[1972].

Atom positions
All the atoms were in general positions. The value of 0.2274 was used for the x coordinate of carbon (5).

Lattice constants
a = 12.929(4) A
b = 13.355(7)
c = 7.976(2)
β = 90.01(3)°
(published values: a=12.9284(41), b=13.3537(68) c=7.9763(17), β=90.010(25)° [Camerman and Camerman, 1972]).

CD cell: a = 12.929, b = 13.355, c = 7.976, β = 90.01, space group $P2_1/a$; a/b = 0.9681, c/b = 0.5972

Volume
1377.2 $A^3$

Density
(measured) 1.39 g/$cm^3$
(calculated) 1.37 g/$cm^3$

Thermal parameters
Isotropic: overall B = 3.0

Scattering factors
$C^0$, $H^0$, $N^0$, $O^0$, $Cl^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.575 \times 10^{-3}$
$I/I_c$ (calculated) = 0.64

Additional pattern
1. MacDonald et al. [1972]

References


Camerman, A. and Camerman, C. (1972). J. Amer. Chem. Soc. 94, 268.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

MacDonald, A., Michaelis, A. F., and Senkowski, B. Z. (1972). In Analytical Profiles of Drug Substances I (1972). (Academic Press, N. Y.), p. 79.


| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | h | k | ℓ | 2θ(°) λ = 1.540598Å |
| 9.28 | 33 | 1 | 1 | 0 | 9.52 |
| 7.96 | 22 | 0 | 0 | 1 | 11.10 |
| 6.84 | 2 | 0 | 1 | 1 | 12.94 |
| 6.67 | 9 | 0 | 2 | 0 | 13.26 |
| 6.46 | 31 | 2 | 0 | 0 | 13.70 |
| 6.05 | 6 | -1 | 1 | 1 | 14.64 |
| 5.93 | 1 | 1 | 2 | 0 | 14.92 |
| 5.12 | 11 | 0 | 2 | 1 | 17.32 |
| 5.02 | 20 | 2 | 0 | 1 | 17.66 |
| 4.70 | 100 | -2 | 1 | 1 | 18.88 |
| 4.64 | 77 | 2 | 2 | 0 | 19.10 |
| 4.21 | 3 | 1 | 3 | 0 | 21.10 |
| 4.10 | 5 | 3 | 1 | 0 | 21.66 |
| 4.01 | 16 | -2 | 2 | 1+ | 22.14 |
| 3.887 | 84 | 0 | 3 | 1 | 22.86 |
| 3.821 | 5 | 0 | 1 | 2 | 23.26 |
| 3.720 | 41 | 1 | 3 | 1+ | 23.90 |
| 3.645 | 12 | -3 | 1 | 1 | 24.40 |
| 3.619 | 21 | 3 | 2 | 0 | 24.58 |
| 3.394 | 6 | 2 | 0 | 2 | 26.24 |
| 3.331 | 16 | -2 | 3 | 1+ | 26.74 |
| 3.309 | 9 | 1 | 2 | 2 | 26.92 |
| 3.297 | 11 | -3 | 2 | 1+ | 27.02 |
| 3.232 | 12 | 1 | 4 | 0 | 27.58 |
| 3.140 | 4 | 4 | 1 | 0 | 28.40 |
| 3.079 | 2 | 0 | 4 | 1 | 28.98 |
| 3.026 | 14 | -2 | 2 | 2+ | 29.50 |
| 2.996 | 23 | 1 | 4 | 1+ | 29.80 |
| 2.967 | 4 | 2 | 4 | 0 | 30.10 |
| 2.923 | 11 | -4 | 1 | 1+ | 30.56 |
| 2.886 | 15 | -3 | 3 | 1+ | 30.96 |
| 2.779 | 6 | -2 | 4 | 1 | 32.18 |
| 2.733 | 1 | 4 | 2 | 1 | 32.74 |
| 2.698 | 5 | 2 | 3 | 2+ | 33.18 |
| 2.681 | 8 | -3 | 2 | 2 | 33.40 |
| 2.639 | 3 | 3 | 4 | 0 | 33.94 |
| 2.556 | 1 | 0 | 4 | 2+ | 35.08 |
| 2.538 | 1 | 5 | 1 | 0 | 35.34 |
| 2.510 | 5 | 1 | 4 | 2+ | 35.74 |
| 2.506 | 5 | -3 | 4 | 1+ | 35.80 |
| 2.485 | 2 | 1 | 5 | 1+ | 36.12 |
| 2.458 | 1 | 2 | 0 | 3+ | 36.52 |
| 2.418 | 6 | -2 | 1 | 3+ | 37.16 |
| 2.413 | 7 | 5 | 2 | 0 | 37.24 |
| 2.379 | 3 | 2 | 4 | 2+ | 37.78 |
| 2.358 | 4 | 2 | 5 | 1+ | 38.14 |
| 2.352 | 4 | -4 | 2 | 2+ | 38.24 |
| 2.308 | 2 | 2 | 2 | 3+ | 39.00 |
| 2.270 | 1 | 3 | 5 | 0 | 39.68 |
| 2.248 | 2 | -1 | 3 | 3+ | 40.08 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | h | k | ℓ | 2θ(°) λ = 1.540598Å |
| 2.230 | 3 | -3 | 1 | 3+ | 40.42 |
| 2.183 | 6 | 3 | 5 | 1+ | 41.32 |
| 2.152 | 4 | -5 | 3 | 1+ | 41.94 |
| 2.144 | 3 | 3 | 2 | 3+ | 42.12 |
| 2.127 | 2 | 6 | 1 | 0 | 42.46 |
| 2.099 | 2 | -2 | 5 | 2+ | 43.06 |
| 2.080 | 2 | 0 | 4 | 3+ | 43.48 |
| 2.063 | 4 | -5 | 2 | 2+ | 43.84 |
| 2.059 | 3 | 4 | 5 | 0+ | 43.94 |
| 2.016 | 1 | 3 | 3 | 3+ | 44.92 |
| 2.007 | 4 | -4 | 4 | 2+ | 45.14 |
| 1.986 | 2 | 6 | 2 | 1 | 45.64 |
| 1.980 | 2 | -5 | 4 | 1+ | 45.78 |
| 1.972 | 5 | 0 | 1 | 4+ | 45.98 |
| 1.950 | 2 | 5 | 3 | 2+ | 46.54 |
| 1.922 | 1 | 1 | 6 | 2 | 47.26 |
| 1.910 | 1 | 0 | 2 | 4 | 47.56 |
| 1.895 | 1 | -6 | 0 | 2 | 47.96 |
| 1.885 | 4 | 0 | 5 | 3+ | 48.24 |
| 1.873 | 2 | 3 | 4 | 3+ | 48.56 |
| 1.865 | 2 | -4 | 3 | 3+ | 48.80 |
| 1.836 | 1 | -5 | 1 | 3+ | 49.60 |
| 1.830 | 2 | 2 | 7 | 0+ | 49.80 |
| 1.819 | 1 | 5 | 4 | 2+ | 50.10 |
| 1.809 | 3 | 2 | 5 | 3 | 50.40 |
| 1.780 | 3 | 7 | 2 | 0+ | 51.28 |
| 1.748 | 1 | -2 | 3 | 4+ | 52.28 |
| 1.721 | 1 | 0 | 7 | 2 | 53.18 |
| 1.706 | 1 | 7 | 3 | 0+ | 53.68 |
| 1.697 | 1 | -4 | 0 | 4+ | 53.98 |
| 1.684 | 1 | -5 | 5 | 2+ | 54.44 |
| 1.665 | 2 | 4 | 6 | 2+ | 55.10 |
| 1.650 | 1 | -2 | 6 | 3+ | 55.66 |
| 1.621 | 1 | -1 | 8 | 1+ | 56.74 |
| 1.598 | 1 | -3 | 7 | 2+ | 57.64 |
| 1.584 | 1 | 2 | 8 | 1+ | 58.18 |
| 1.549 | 1 | -2 | 0 | 5+ | 59.66 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | h | k | ℓ | 2θ(°) λ = 1.540598Å |
| 9.29 | 34 | 1 | 1 | 0 | 9.51 |
| 7.98 | 23 | 0 | 0 | 1 | 11.08 |
| 6.85 | 2 | 0 | 1 | 1 | 12.92 |
| 6.68 | 9 | 0 | 2 | 0 | 13.25 |
| 6.46 | 37 | 2 | 0 | 0 | 13.69 |
| 6.05 | 6 | -1 | 1 | 1 | 14.63 |
| 5.93 | 1 | 1 | 2 | 0 | 14.92 |
| 5.12 | 12 | 0 | 2 | 1 | 17.31 |
| 5.02 | 21 | 2 | 0 | 1 | 17.65 |
| 4.76 | 1 | -1 | 2 | 1 | 18.62 |
| 4.76 | 2 | 1 | 2 | 1 | 18.63 |
| 4.70 | 100 | -2 | 1 | 1 | 18.86 |
| 4.70 | 8 | 2 | 1 | 1 | 18.86 |
| 4.64 | 79 | 2 | 2 | 0 | 19.09 |
| 4.21 | 3 | 1 | 3 | 0 | 21.09 |
| 4.10 | 5 | 3 | 1 | 0 | 21.65 |
| 4.01 | 13 | -2 | 2 | 1 | 22.13 |
| 4.01 | 5 | 2 | 2 | 1 | 22.13 |
| 3.887 | 100 | 0 | 3 | 1 | 22.86 |
| 3.821 | 3 | 0 | 1 | 2 | 23.26 |
| 3.723 | 15 | -1 | 3 | 1 | 23.88 |
| 3.722 | 32 | 1 | 3 | 1 | 23.89 |
| 3.666 | 3 | 2 | 3 | 0 | 24.26 |
| 3.664 | 1 | 1 | 1 | 2 | 24.27 |
| 3.648 | 9 | -3 | 1 | 1 | 24.38 |
| 3.621 | 23 | 3 | 2 | 0 | 24.56 |
| 3.394 | 7 | 2 | 0 | 2 | 26.24 |
| 3.331 | 10 | -2 | 3 | 1 | 26.74 |
| 3.331 | 8 | 2 | 3 | 1 | 26.74 |
| 3.310 | 5 | 1 | 2 | 2 | 26.92 |
| 3.297 | 5 | -3 | 2 | 1 | 27.02 |
| 3.297 | 2 | 3 | 2 | 1 | 27.02 |
| 3.290 | 3 | -2 | 1 | 2 | 27.08 |
| 3.289 | 1 | 2 | 1 | 2 | 27.09 |
| 3.233 | 13 | 1 | 4 | 0 | 27.57 |
| 3.142 | 4 | 4 | 1 | 0 | 28.39 |
| 3.096 | 1 | 3 | 3 | 0 | 28.81 |
| 3.080 | 2 | 0 | 4 | 1 | 28.97 |
| 3.026 | 11 | -2 | 2 | 2 | 29.50 |
| 3.025 | 6 | 2 | 2 | 2 | 29.50 |
| 2.996 | 7 | -1 | 4 | 1 | 29.80 |
| 2.996 | 12 | 1 | 4 | 1 | 29.80 |
| 2.995 | 8 | 4 | 0 | 1 | 29.80 |
| 2.966 | 3 | 2 | 4 | 0 | 30.10 |
| 2.923 | 7 | -4 | 1 | 1 | 30.56 |
| 2.923 | 6 | 4 | 1 | 1 | 30.56 |
| 2.895 | 6 | -1 | 3 | 2 | 30.86 |
| 2.887 | 8 | -3 | 3 | 1 | 30.95 |
| 2.886 | 8 | 3 | 3 | 1 | 30.96 |
| 2.780 | 7 | -2 | 4 | 1 | 32.17 |

Diazepam, $C_{16}H_{13}ClN_2O$ -(Continued)

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.780 | 1 | 2 | 4 | 1 | 32.17 |
| 2.733 | 1 | 4 | 2 | 1 | 32.74 |
| 2.699 | 2 | -2 | 3 | 2 | 33.16 |
| 2.699 | 3 | 2 | 3 | 2 | 33.17 |
| 2.681 | 9 | -3 | 2 | 2 | 33.39 |
| 2.639 | 3 | 3 | 4 | 0 | 33.94 |
| 2.539 | 1 | 5 | 1 | 0 | 35.33 |
| 2.511 | 4 | 1 | 4 | 2 | 35.73 |
| 2.511 | 1 | 4 | 0 | 2 | 35.73 |
| 2.506 | 1 | -3 | 4 | 1 | 35.81 |
| 2.506 | 1 | 3 | 4 | 1 | 35.81 |
| 2.485 | 2 | 1 | 5 | 1 | 36.11 |
| 2.459 | 1 | 2 | 0 | 3 | 36.52 |
| 2.419 | 3 | 5 | 1 | 1 | 37.14 |
| 2.418 | 4 | -2 | 1 | 3 | 37.15 |
| 2.418 | 1 | 2 | 1 | 3 | 37.15 |
| 2.411 | 4 | 5 | 2 | 0 | 37.26 |
| 2.380 | 1 | -2 | 4 | 2 | 37.76 |
| 2.380 | 2 | 2 | 4 | 2 | 37.77 |
| 2.358 | 2 | -2 | 5 | 1 | 38.13 |
| 2.358 | 4 | 2 | 5 | 1 | 38.13 |
| 2.351 | 2 | -4 | 2 | 2 | 38.26 |
| 2.307 | 1 | 2 | 2 | 3 | 39.01 |
| 2.270 | 2 | 3 | 5 | 0 | 39.67 |
| 2.248 | 1 | -1 | 3 | 3 | 40.08 |
| 2.231 | 2 | -3 | 1 | 3 | 40.39 |
| 2.230 | 1 | -4 | 4 | 1 | 40.42 |
| 2.230 | 1 | 4 | 4 | 1 | 40.42 |
| 2.194 | 2 | 1 | 6 | 0 | 41.12 |
| 2.187 | 1 | -1 | 5 | 2 | 41.24 |
| 2.187 | 1 | 4 | 3 | 2 | 41.25 |
| 2.184 | 1 | -3 | 5 | 1 | 41.31 |
| 2.184 | 6 | 3 | 5 | 1 | 41.31 |
| 2.153 | 3 | -5 | 3 | 1 | 41.93 |
| 2.153 | 1 | 5 | 3 | 1 | 41.93 |
| 2.152 | 1 | 2 | 3 | 3 | 41.94 |
| 2.143 | 1 | -3 | 2 | 3 | 42.13 |
| 2.143 | 2 | 3 | 2 | 3 | 42.13 |
| 2.127 | 3 | 6 | 1 | 0 | 42.46 |
| 2.099 | 2 | -2 | 5 | 2 | 43.06 |
| 2.099 | 1 | 2 | 5 | 2 | 43.06 |
| 2.080 | 1 | 0 | 4 | 3 | 43.48 |
| 2.064 | 3 | -5 | 2 | 2 | 43.84 |
| 2.063 | 1 | 5 | 2 | 2 | 43.84 |
| 2.059 | 1 | 4 | 5 | 0 | 43.94 |
| 2.055 | 1 | 6 | 1 | 1 | 44.02 |
| 2.007 | 4 | -4 | 4 | 2 | 45.14 |
| 2.007 | 1 | 4 | 4 | 2 | 45.15 |
| 1.986 | 2 | 6 | 2 | 1 | 45.64 |
| 1.973 | 2 | -3 | 5 | 2 | 45.96 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.973 | 2 | 3 | 5 | 2 | 45.96 |
| 1.972 | 3 | 0 | 1 | 4 | 45.98 |
| 1.950 | 1 | 5 | 3 | 2 | 46.53 |
| 1.950 | 1 | 1 | 1 | 4 | 46.55 |
| 1.922 | 2 | 1 | 6 | 2 | 47.25 |
| 1.911 | 1 | 0 | 2 | 4 | 47.55 |
| 1.896 | 1 | -6 | 0 | 2 | 47.94 |
| 1.890 | 1 | -1 | 2 | 4 | 48.10 |
| 1.885 | 2 | -6 | 3 | 1 | 48.25 |
| 1.884 | 2 | 0 | 5 | 3 | 48.26 |
| 1.873 | 2 | 3 | 4 | 3 | 48.57 |
| 1.865 | 1 | -4 | 3 | 3 | 48.80 |
| 1.836 | 1 | -5 | 1 | 3 | 49.61 |
| 1.830 | 1 | 2 | 7 | 0 | 49.79 |
| 1.829 | 1 | 4 | 5 | 2 | 49.80 |
| 1.819 | 1 | 5 | 4 | 2 | 50.10 |
| 1.809 | 3 | 2 | 5 | 3 | 50.41 |
| 1.787 | 1 | -4 | 6 | 1 | 51.08 |
| 1.780 | 3 | 7 | 2 | 0 | 51.28 |
| 1.721 | 1 | 0 | 7 | 2 | 53.18 |
| 1.706 | 1 | 7 | 3 | 0 | 53.68 |
| 1.684 | 1 | -5 | 5 | 2 | 54.44 |
| 1.666 | 1 | 4 | 6 | 2 | 55.09 |
| 1.650 | 1 | -2 | 6 | 3 | 55.65 |
| 1.621 | 1 | -1 | 8 | 1 | 56.74 |
| 1.584 | 1 | 2 | 8 | 1 | 58.19 |
| 1.549 | 1 | -2 | 0 | 5 | 59.65 |

# (N,N)-Dimethyltryptamine, $C_{12}H_{16}N_2$

Synonyms
DMT, 3-[2-(dimethylamino)-ethyl]indole

Structure
Monoclinic, $P2_1/c$ (14), Z = 8. The structure was determined by Falkenberg [1972].

Atom positions [ibid.]
All the atoms were in general positions, with 2 molecules in the asymmetric unit.

Polymorphism [ibid.]
The batch of the material described here also contained crystals of an entirely different polymorph. The latter could easily be distinguished by its optical properties and crystal shape, and had the monoclinic space group $P2_1/c$ with Z = 4.

Lattice constants [ibid.]
a = 12.99(1) A
b = 12.08(1)
c = 18.38(2)
β = 127.85(1)°

CD cell: a = 14.61, b = 12.08, c = 12.99, β = 96.73°, space group $P2_1/n$; a/b = 1.2098, c/b = 1.0753

Volume
2278. $A^3$

Density
(measured) 1.080 $g/cm^3$
(calculated) 1.098 $g/cm^3$

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
$C^0$, $H^0$, $N^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.321 \times 10^{-3}$
$I/I_c$ (calculated) = 0.39

Additional pattern
1. Folen [1975].

References

Falkenberg, G. (1972). Acta Crystallogr. B28, 3075.
Folen, V. A. (1975). J. Forens. Sci. 20, 348.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
|---|---|---|---|---|---|
| 9.28 | 47 | 0 | 1 | 1 | 9.52 |
| 8.80 | 14 | -1 | 1 | 1 | 10.04 |
| 7.81 | 4 | 1 | 1 | 0 | 11.32 |
| 7.27 | 15 | -1 | 1 | 2+ | 12.16 |
| 6.45 | 45 | -2 | 0 | 2 | 13.72 |
| 6.21 | 100 | 0 | 1 | 2 | 14.24 |
| 6.04 | 49 | 0 | 2 | 0 | 14.66 |
| 5.68 | 7 | -2 | 1 | 2 | 15.58 |
| 5.57 | 11 | 0 | 2 | 1 | 15.90 |
| 5.49 | 51 | -2 | 1 | 1 | 16.14 |
| 5.40 | 7 | -1 | 1 | 3 | 16.40 |
| 5.20 | 14 | 1 | 2 | 0 | 17.04 |
| 5.12 | 22 | 2 | 0 | 0+ | 17.30 |
| 5.04 | 8 | -1 | 2 | 2 | 17.60 |
| 4.71 | 35 | 1 | 0 | 2 | 18.82 |
| 4.64 | 48 | 0 | 2 | 2 | 19.12 |
| 4.56 | 7 | -2 | 0 | 4 | 19.46 |
| 4.48 | 68 | 1 | 2 | 1+ | 19.80 |
| 4.41 | 17 | -2 | 2 | 2 | 20.14 |
| 4.36 | 31 | -1 | 0 | 4 | 20.34 |
| 4.31 | 61 | -2 | 2 | 1 | 20.58 |
| 4.26 | 99 | -2 | 1 | 4+ | 20.82 |
| 4.13 | 73 | -2 | 2 | 3 | 21.52 |
| 4.05 | 6 | -3 | 1 | 3 | 21.92 |
| 4.00 | 22 | -3 | 0 | 4 | 22.22 |
| 3.89 | 12 | 2 | 1 | 1 | 22.86 |
| 3.79 | 35 | -3 | 1 | 4 | 23.44 |
| 3.71 | 12 | 1 | 2 | 2+ | 23.94 |
| 3.64 | 16 | -2 | 2 | 4 | 24.44 |
| 3.53 | 11 | -1 | 2 | 4 | 25.18 |
| 3.51 | 23 | -2 | 1 | 5+ | 25.36 |
| 3.45 | 3 | 1 | 3 | 1 | 25.84 |
| 3.42 | 7 | 3 | 0 | 0 | 26.06 |
| 3.37 | 14 | -2 | 3 | 1+ | 26.40 |
| 3.33 | 10 | -3 | 2 | 4 | 26.72 |
| 3.28 | 12 | -3 | 2 | 1+ | 27.18 |
| 3.22 | 11 | -4 | 0 | 4+ | 27.72 |
| 3.17 | 2 | 2 | 3 | 0 | 28.16 |
| 3.11 | 14 | -4 | 1 | 4 | 28.64 |
| 3.10 | 8 | 1 | 2 | 3+ | 28.82 |
| 3.06 | 3 | 1 | 3 | 2 | 29.14 |
| 3.02 | 6 | -2 | 0 | 6+ | 29.60 |
| 2.976 | 3 | -4 | 1 | 5+ | 30.00 |
| 2.951 | 5 | -3 | 1 | 6+ | 30.26 |
| 2.919 | 2 | 2 | 2 | 2 | 30.60 |
| 2.864 | 6 | 3 | 1 | 1 | 31.20 |
| 2.845 | 3 | -4 | 2 | 4+ | 31.42 |
| 2.826 | 3 | -4 | 0 | 6+ | 31.64 |
| 2.746 | 4 | -4 | 2 | 2+ | 32.58 |
| 2.712 | 10 | -2 | 3 | 5+ | 33.00 |

| Calculated Pattern (Peak heights) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.651 | 2 | -3 | 3 | 5+ | 33.78 |
| 2.618 | 4 | 1 | 2 | 4 | 34.22 |
| 2.606 | 5 | 3 | 3 | 0+ | 34.38 |
| 2.560 | 6 | -4 | 2 | 6+ | 35.02 |
| 2.483 | 1 | -2 | 1 | 7 | 36.14 |
| 2.464 | 3 | -3 | 4 | 2 | 36.44 |
| 2.448 | 3 | -4 | 3 | 2 | 36.68 |
| 2.443 | 3 | -4 | 3 | 5 | 36.76 |
| 2.413 | 3 | -2 | 3 | 6 | 37.24 |
| 2.382 | 2 | 1 | 1 | 5+ | 37.74 |
| 2.360 | 2 | 4 | 2 | 0 | 38.10 |
| 2.348 | 2 | 3 | 2 | 2 | 38.30 |
| 2.303 | 5 | -5 | 1 | 7 | 39.08 |
| 2.262 | 1 | -2 | 5 | 2 | 39.82 |
| 2.255 | 1 | -1 | 4 | 5+ | 39.94 |
| 2.241 | 3 | -4 | 1 | 8+ | 40.20 |
| 2.239 | 3 | 2 | 4 | 2 | 40.24 |
| 2.221 | 1 | -2 | 5 | 3 | 40.58 |
| 2.200 | 2 | -3 | 3 | 7+ | 41.00 |
| 2.186 | 2 | 2 | 5 | 0+ | 41.26 |
| 2.173 | 1 | -1 | 2 | 7+ | 41.52 |
| 2.153 | 2 | -4 | 4 | 2+ | 41.92 |
| 2.139 | 2 | -5 | 1 | 8+ | 42.22 |
| 2.134 | 2 | -6 | 0 | 4+ | 42.32 |
| 2.114 | 1 | -6 | 1 | 6+ | 42.74 |
| 2.098 | 1 | -6 | 1 | 4+ | 43.08 |
| 2.063 | 1 | -4 | 4 | 6+ | 43.84 |
| 2.055 | 1 | 1 | 1 | 6+ | 44.02 |
| 2.039 | 1 | -1 | 4 | 6+ | 44.40 |
| 2.027 | 2 | -5 | 3 | 7+ | 44.68 |
| 2.007 | 2 | 1 | 5 | 3+ | 45.14 |
| 1.984 | 2 | -4 | 3 | 8+ | 45.70 |
| 1.967 | 1 | -1 | 5 | 5+ | 46.10 |
| 1.959 | 2 | 3 | 0 | 4 | 46.30 |
| 1.943 | 1 | 5 | 2 | 0+ | 46.72 |
| 1.934 | 1 | -4 | 2 | 9+ | 46.94 |
| 1.922 | 1 | -2 | 6 | 2+ | 47.26 |
| 1.897 | 2 | -2 | 6 | 3+ | 47.92 |
| 1.874 | 2 | 2 | 6 | 0+ | 48.54 |
| 1.856 | 2 | -6 | 3 | 7+ | 49.04 |
| 1.852 | 2 | 1 | 6 | 2 | 49.16 |
| 1.843 | 1 | 0 | 3 | 7+ | 49.40 |
| 1.824 | 1 | -5 | 0 | 10+ | 49.96 |
| 1.798 | 2 | -3 | 3 | 9+ | 50.72 |
| 1.783 | 1 | 2 | 1 | 6+ | 51.20 |
| 1.761 | 1 | -7 | 2 | 7+ | 51.88 |
| 1.727 | 1 | -7 | 2 | 8+ | 52.98 |
| 1.678 | 1 | 0 | 7 | 2+ | 54.66 |
| 1.670 | 1 | -4 | 3 | 10+ | 54.94 |
| 1.659 | 1 | -7 | 0 | 10+ | 55.34 |
| 1.642 | 1 | -4 | 1 | 11+ | 55.94 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 9.28 | 46 | 0 | 1 | 1 | 9.52 |
| 9.13 | 2 | -1 | 0 | 2 | 9.68 |
| 8.82 | 14 | -1 | 1 | 1 | 10.02 |
| 7.82 | 4 | 1 | 1 | 0 | 11.31 |
| 7.28 | 11 | -1 | 1 | 2 | 12.15 |
| 7.26 | 5 | 0 | 0 | 2 | 12.19 |
| 6.45 | 45 | -2 | 0 | 2 | 13.72 |
| 6.22 | 100 | 0 | 1 | 2 | 14.23 |
| 6.04 | 47 | 0 | 2 | 0 | 14.65 |
| 5.69 | 6 | -2 | 1 | 2 | 15.56 |
| 5.58 | 7 | 0 | 2 | 1 | 15.88 |
| 5.49 | 49 | -2 | 1 | 1 | 16.12 |
| 5.47 | 7 | -1 | 2 | 1 | 16.19 |
| 5.40 | 4 | -1 | 1 | 3 | 16.42 |
| 5.20 | 12 | 1 | 2 | 0 | 17.02 |
| 5.13 | 18 | 2 | 0 | 0 | 17.28 |
| 5.12 | 5 | -2 | 1 | 3 | 17.30 |
| 5.04 | 7 | -1 | 2 | 2 | 17.59 |
| 4.72 | 3 | 2 | 1 | 0 | 18.78 |
| 4.71 | 31 | 1 | 0 | 2 | 18.81 |
| 4.64 | 48 | 0 | 2 | 2 | 19.10 |
| 4.56 | 2 | -2 | 0 | 4 | 19.44 |
| 4.49 | 40 | 0 | 1 | 3 | 19.75 |
| 4.48 | 43 | 1 | 2 | 1 | 19.82 |
| 4.41 | 10 | -2 | 2 | 2 | 20.12 |
| 4.36 | 25 | -1 | 0 | 4 | 20.33 |
| 4.32 | 55 | -2 | 2 | 1 | 20.56 |
| 4.27 | 66 | -2 | 1 | 4 | 20.79 |
| 4.27 | 22 | -1 | 2 | 3 | 20.80 |
| 4.26 | 19 | -3 | 0 | 2 | 20.83 |
| 4.13 | 77 | -2 | 2 | 3 | 21.51 |
| 4.10 | 6 | -1 | 1 | 4 | 21.63 |
| 4.05 | 3 | -3 | 1 | 3 | 21.92 |
| 4.02 | 2 | -3 | 1 | 2 | 22.10 |
| 4.00 | 22 | -3 | 0 | 4 | 22.22 |
| 3.89 | 11 | 2 | 1 | 1 | 22.85 |
| 3.80 | 38 | -3 | 1 | 4 | 23.42 |
| 3.78 | 2 | 0 | 2 | 3 | 23.54 |
| 3.72 | 8 | 1 | 2 | 2 | 23.92 |
| 3.72 | 4 | -3 | 1 | 1 | 23.93 |
| 3.64 | 17 | -2 | 2 | 4 | 24.43 |
| 3.63 | 1 | 0 | 0 | 4 | 24.51 |
| 3.54 | 9 | -1 | 2 | 4 | 25.15 |
| 3.51 | 20 | -2 | 1 | 5 | 25.35 |
| 3.50 | 7 | -3 | 2 | 3 | 25.41 |
| 3.47 | 1 | 0 | 1 | 4 | 25.61 |
| 3.45 | 2 | 1 | 3 | 1 | 25.83 |
| 3.42 | 6 | 3 | 0 | 0 | 26.04 |
| 3.40 | 5 | 2 | 2 | 1 | 26.21 |
| 3.38 | 6 | -3 | 1 | 5 | 26.33 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 3.37 | 11 | -2 | 3 | 1 | 26.41 |
| 3.35 | 2 | -1 | 3 | 3 | 26.60 |
| 3.33 | 10 | -3 | 2 | 4 | 26.72 |
| 3.29 | 2 | 3 | 1 | 0 | 27.08 |
| 3.28 | 1 | -2 | 3 | 3 | 27.17 |
| 3.28 | 10 | -3 | 2 | 1 | 27.17 |
| 3.23 | 9 | -4 | 0 | 4 | 27.64 |
| 3.21 | 7 | 2 | 1 | 2 | 27.74 |
| 3.17 | 1 | 2 | 3 | 0 | 28.15 |
| 3.12 | 14 | -4 | 1 | 4 | 28.62 |
| 3.11 | 1 | 0 | 2 | 4 | 28.68 |
| 3.10 | 5 | 1 | 2 | 3 | 28.82 |
| 3.09 | 1 | 0 | 3 | 3 | 28.82 |
| 3.08 | 2 | -4 | 0 | 2 | 28.92 |
| 3.06 | 3 | 1 | 3 | 2 | 29.14 |
| 3.02 | 2 | 0 | 4 | 0 | 29.55 |
| 3.02 | 3 | -2 | 3 | 4 | 29.56 |
| 3.02 | 3 | -2 | 0 | 6 | 29.61 |
| 2.978 | 2 | -4 | 1 | 5 | 29.98 |
| 2.975 | 1 | 3 | 2 | 0 | 30.01 |
| 2.960 | 1 | -1 | 3 | 4 | 30.17 |
| 2.957 | 2 | -1 | 2 | 5 | 30.20 |
| 2.950 | 3 | -3 | 1 | 6 | 30.27 |
| 2.939 | 2 | -3 | 3 | 3 | 30.39 |
| 2.919 | 1 | 2 | 2 | 2 | 30.61 |
| 2.906 | 1 | 1 | 0 | 4 | 30.75 |
| 2.876 | 3 | 2 | 3 | 1 | 31.08 |
| 2.864 | 5 | 3 | 1 | 1 | 31.20 |
| 2.848 | 1 | -4 | 2 | 3 | 31.39 |
| 2.845 | 2 | -4 | 2 | 4 | 31.42 |
| 2.827 | 3 | -4 | 0 | 6 | 31.63 |
| 2.822 | 1 | 0 | 1 | 5 | 31.68 |
| 2.752 | 1 | -4 | 1 | 6 | 32.50 |
| 2.747 | 3 | -4 | 2 | 2 | 32.57 |
| 2.735 | 1 | -2 | 4 | 2 | 32.72 |
| 2.717 | 1 | -3 | 2 | 6 | 32.94 |
| 2.712 | 2 | -2 | 4 | 1 | 33.00 |
| 2.712 | 8 | -2 | 3 | 5 | 33.00 |
| 2.698 | 3 | -2 | 2 | 6 | 33.18 |
| 2.695 | 1 | 0 | 3 | 4 | 33.21 |
| 2.651 | 2 | -3 | 3 | 5 | 33.78 |
| 2.618 | 4 | 1 | 2 | 4 | 34.22 |
| 2.606 | 4 | 3 | 3 | 0 | 34.38 |
| 2.602 | 1 | 2 | 4 | 0 | 34.44 |
| 2.566 | 4 | -3 | 1 | 7 | 34.94 |
| 2.560 | 4 | -4 | 2 | 6 | 35.02 |
| 2.543 | 1 | 1 | 4 | 2 | 35.26 |
| 2.484 | 1 | -2 | 1 | 7 | 36.13 |
| 2.471 | 1 | -3 | 4 | 3 | 36.32 |
| 2.464 | 3 | -3 | 4 | 2 | 36.44 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.449 | 2 | -4 | 3 | 2 | 36.67 |
| 2.443 | 1 | -4 | 3 | 5 | 36.76 |
| 2.413 | 4 | -2 | 3 | 6 | 37.23 |
| 2.382 | 1 | 1 | 1 | 5 | 37.74 |
| 2.360 | 2 | 4 | 2 | 0 | 38.09 |
| 2.348 | 1 | 3 | 2 | 2 | 38.31 |
| 2.303 | 5 | -5 | 1 | 7 | 39.08 |
| 2.262 | 1 | -2 | 5 | 2 | 39.81 |
| 2.243 | 1 | -1 | 5 | 3 | 40.18 |
| 2.242 | 1 | -4 | 1 | 8 | 40.19 |
| 2.238 | 2 | 2 | 4 | 2 | 40.26 |
| 2.222 | 1 | -2 | 5 | 3 | 40.57 |
| 2.204 | 1 | -4 | 4 | 4 | 40.91 |
| 2.199 | 2 | -3 | 3 | 7 | 41.00 |
| 2.158 | 1 | -4 | 4 | 2 | 41.83 |
| 2.139 | 1 | -5 | 1 | 8 | 42.22 |
| 2.134 | 1 | -4 | 2 | 8 | 42.31 |
| 2.131 | 1 | -6 | 0 | 4 | 42.39 |
| 2.098 | 1 | -6 | 1 | 4 | 43.08 |
| 2.039 | 1 | -1 | 4 | 6 | 44.40 |
| 2.027 | 1 | -5 | 3 | 7 | 44.67 |
| 2.007 | 1 | 1 | 5 | 3 | 45.14 |
| 1.985 | 1 | -4 | 3 | 8 | 45.67 |
| 1.983 | 1 | -1 | 1 | 8 | 45.71 |
| 1.960 | 2 | 3 | 0 | 4 | 46.30 |
| 1.934 | 1 | -4 | 2 | 9 | 46.94 |
| 1.898 | 1 | -6 | 2 | 8 | 47.90 |
| 1.897 | 2 | -2 | 6 | 3 | 47.92 |
| 1.874 | 1 | 2 | 6 | 0 | 48.54 |
| 1.856 | 1 | -6 | 3 | 7 | 49.04 |
| 1.852 | 1 | 1 | 6 | 2 | 49.17 |
| 1.799 | 1 | -6 | 2 | 9 | 50.70 |
| 1.798 | 1 | -3 | 3 | 9 | 50.72 |
| 1.783 | 1 | 2 | 1 | 6 | 51.21 |
| 1.763 | 1 | -7 | 2 | 7 | 51.82 |
| 1.727 | 1 | -7 | 2 | 8 | 52.98 |
| 1.679 | 1 | 0 | 7 | 2 | 54.62 |
| 1.670 | 1 | -7 | 2 | 9 | 54.92 |
| 1.670 | 1 | -4 | 3 | 10 | 54.95 |

# Methapyrilene hydrochloride, $C_{14}H_{20}ClN_3S$

Synonyms
1. 2-[(2)-dimethylaminoethyl-2-thenylamino]-pyridine hydrochloride
2. thenylpyramine hydrochloride

Structure
Monoclinic, $P2_1/c$ (14), Z = 8. The structure was determined by Clark and Palenik [1972]. There were two molecules in the asymmetric unit and in one of them the thiophene ring was disordered; one sulfur and one carbon atom shared occupancy of each of 2 sites, on an approximately equal basis.

Atom positions
Three hydrogen atoms on the disordered thiophene ring were omitted from the refinement and their positions not determined. All other atoms were in general positions.

Lattice constants
a = 10.937(3) Å
b = 10.418(3)
c = 28.258(8)
β = 106.21(2)°
(published values: a = 10.936, b = 10.417
c = 28.256, β = 106.21° [Clark and Palenik, 1972]

CD cell: a = 27.305, b = 10.418, c = 10.937, β = 96.41°, space group $P2_1/n$, a/b = 2.6209, c/b = 1.0498

Volume
3091.8 Å$^3$

Density
(measured) 1.273 g/cm$^3$
(calculated) 1.280 g/cm$^3$

Thermal parameters
Isotropic: overall B = 5.0

Scattering factors
$C^0$, $H^0$, $Cl^0$, $N^0$, $S^0$ [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.213 \times 10^{-3}$
$I/I_c$ (calculated) = 0.35

Additional pattern
1. PDF 12-872 [Rose and Williams, 1959]

References

Clark, G. R. and Palenik, G. J. (1972). J. Amer. Chem. Soc. 94, 4005.

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Rose, H. A. and Williams, J. G. (1959). J. Amer. Pharm. Ass. 48, 487.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 9.71 | 3 | 0 1 1 | 9.10 |
| 8.26 | 7 | 0 1 2 | 10.70 |
| 7.52 | 60 | -1 1 1 | 11.76 |
| 7.10 | 10 | -1 1 2 | 12.46 |
| 6.79 | 26 | 1 1 1* | 13.02 |
| 6.59 | 3 | -1 0 4 | 13.42 |
| 6.37 | 5 | -1 1 3 | 13.90 |
| 6.01 | 1 | 1 1 2 | 14.72 |
| 5.68 | 13 | 0 1 4 | 15.58 |
| 5.58 | 2 | -1 1 4 | 15.88 |
| 5.43 | 5 | -2 0 2 | 16.30 |
| 5.21 | 40 | 0 2 0 | 17.02 |
| 4.85 | 93 | -2 0 4* | 18.26 |
| 4.69 | 20 | 2 1 0 | 18.92 |
| 4.59 | 8 | -1 2 2 | 19.34 |
| 4.52 | 47 | 0 0 6 | 19.62 |
| 4.37 | 24 | -1 2 3 | 20.30 |
| 4.25 | 7 | -1 1 6 | 20.90 |
| 4.13 | 100 | 2 1 2* | 21.52 |
| 4.02 | 37 | -2 0 6* | 22.10 |
| 3.757 | 67 | -2 1 6* | 23.66 |
| 3.684 | 53 | 2 0 4* | 24.14 |
| 3.553 | 38 | -2 2 4 | 25.04 |
| 3.469 | 10 | -1 2 6 | 25.66 |
| 3.437 | 5 | -2 1 7* | 25.90 |
| 3.401 | 15 | -3 1 1* | 26.18 |
| 3.341 | 7 | 1 2 5* | 26.66 |
| 3.300 | 4 | -2 0 8* | 27.00 |
| 3.269 | 2 | -1 3 2 | 27.26 |
| 3.225 | 4 | 0 1 8 | 27.64 |
| 3.186 | 17 | 1 1 7* | 27.98 |
| 3.144 | 23 | -2 1 8 | 28.36 |
| 3.091 | 2 | 0 3 4 | 28.86 |
| 3.064 | 2 | 1 2 6* | 29.12 |
| 3.008 | 20 | 2 2 4* | 29.68 |
| 2.974 | 16 | -3 2 3* | 30.02 |
| 2.912 | 21 | 2 1 6 | 30.68 |
| 2.879 | 6 | 3 1 3* | 31.04 |
| 2.850 | 2 | -3 2 5 | 31.36 |
| 2.834 | 3 | 2 3 1 | 31.54 |
| 2.788 | 5 | -2 2 8 | 32.08 |
| 2.746 | 3 | 0 3 6* | 32.58 |
| 2.736 | 3 | -2 3 5 | 32.70 |
| 2.715 | 9 | -4 0 4* | 32.96 |
| 2.688 | 2 | -1 2 9 | 33.30 |
| 2.679 | 2 | 2 1 7 | 33.42 |
| 2.651 | 2 | -2 1 10 | 33.78 |
| 2.626 | 6 | -1 3 7* | 34.12 |
| 2.623 | 6 | 1 1 9* | 34.16 |
| 2.601 | 7 | -2 2 9* | 34.46 |

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 2.546 | 9 | 3 1 5* | 35.22 |
| 2.527 | 6 | 2 3 4* | 35.50 |
| 2.502 | 6 | 1 4 1* | 35.86 |
| 2.475 | 7 | -1 4 3* | 36.26 |
| 2.449 | 3 | 4 0 2* | 36.66 |
| 2.430 | 7 | 0 4 4* | 36.96 |
| 2.409 | 3 | 1 3 7* | 37.30 |
| 2.391 | 4 | 1 4 3* | 37.58 |
| 2.388 | 4 | -3 2 9* | 37.64 |
| 2.367 | 2 | -4 1 8 | 37.98 |
| 2.346 | 4 | 3 2 5* | 38.34 |
| 2.332 | 4 | -4 2 6* | 38.58 |
| 2.301 | 1 | -1 2 11* | 39.12 |
| 2.285 | 2 | 2 3 6* | 39.40 |
| 2.276 | 2 | 0 3 9 | 39.56 |
| 2.272 | 2 | -1 4 6* | 39.64 |
| 2.262 | 1 | 0 0 12* | 39.82 |
| 2.246 | 1 | 3 1 7* | 40.12 |
| 2.222 | 3 | -4 0 10* | 40.56 |
| 2.213 | 3 | 1 1 11* | 40.74 |
| 2.194 | 1 | 2 4 3* | 41.10 |
| 2.175 | 3 | 2 0 10 | 41.48 |
| 2.152 | 2 | -2 3 10 | 41.94 |
| 2.138 | 4 | -4 3 2* | 42.24 |
| 2.133 | 4 | 1 3 9 | 42.34 |
| 2.128 | 4 | 2 1 10* | 42.44 |
| 2.124 | 4 | -2 2 12* | 42.52 |
| 2.094 | 1 | 3 3 5* | 43.16 |
| 2.069 | 2 | -3 4 5 | 43.72 |
| 2.063 | 3 | 4 2 4* | 43.86 |
| 2.044 | 2 | 1 5 0* | 44.28 |
| 2.038 | 2 | -1 5 2* | 44.42 |
| 2.030 | 3 | 0 5 3* | 44.60 |
| 2.010 | 2 | -2 0 14* | 45.08 |
| 1.999 | 5 | 4 1 6 | 45.32 |
| 1.982 | 1 | -3 4 7 | 45.74 |
| 1.973 | 3 | -2 1 14* | 45.96 |
| 1.947 | 2 | 4 3 3* | 46.62 |
| 1.939 | 3 | 0 0 14* | 46.82 |
| 1.933 | 2 | -2 3 12* | 46.96 |
| 1.929 | 2 | -3 4 8 | 47.08 |
| 1.917 | 2 | 3 3 7* | 47.38 |
| 1.890 | 3 | 2 5 2 | 48.10 |
| 1.872 | 2 | -5 2 9* | 48.60 |
| 1.863 | 2 | 2 1 12 | 48.84 |
| 1.858 | 2 | -3 3 12 | 48.98 |
| 1.850 | 1 | 4 4 0* | 49.22 |
| 1.843 | 2 | -1 1 15* | 49.42 |
| 1.822 | 3 | -5 3 1* | 50.02 |
| 1.801 | 2 | -3 1 15* | 50.64 |

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 1.795 | 3 | -4 1 14* | 50.84 |
| 1.791 | 2 | 1 4 10* | 50.96 |
| 1.775 | 3 | -3 3 13* | 51.44 |
| 1.770 | 3 | -6 0 8* | 51.60 |
| 1.750 | 1 | 6 0 0* | 52.22 |
| 1.744 | 2 | -3 4 11* | 52.42 |
| 1.740 | 2 | 4 2 8* | 52.56 |
| 1.720 | 1 | 3 4 7* | 53.22 |
| 1.710 | 2 | -6 2 6* | 53.54 |
| 1.697 | 1 | -1 6 3* | 54.00 |
| 1.694 | 1 | -3 3 14* | 54.10 |
| 1.668 | 2 | 4 0 10* | 55.00 |
| 1.659 | 1 | -2 5 10* | 55.34 |
| 1.655 | 2 | -1 6 5* | 55.48 |
| 1.619 | 1 | -6 2 10* | 56.84 |
| 1.612 | 1 | 2 5 8* | 57.08 |
| 1.588 | 2 | 4 5 2* | 58.02 |
| 1.559 | 1 | 1 4 13* | 59.22 |
| 1.555 | 1 | -4 1 17* | 59.38 |
| 1.550 | 1 | -4 3 15* | 59.58 |
| 1.547 | 1 | -7 1 5* | 59.74 |

Calculated Pattern (Integrated)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 9.73 | 3 | 0 1 1 | 9.09 |
| 8.26 | 8 | 0 1 2 | 10.70 |
| 7.52 | 72 | -1 1 1 | 11.76 |
| 7.40 | 5 | 1 1 0 | 11.96 |
| 7.11 | 11 | -1 1 2 | 12.44 |
| 6.83 | 1 | 0 1 3 | 12.95 |
| 6.80 | 20 | 1 1 1 | 13.00 |
| 6.78 | 13 | 0 0 4 | 13.04 |
| 6.60 | 2 | -1 0 4 | 13.41 |
| 6.37 | 6 | -1 1 3 | 13.89 |
| 6.02 | 1 | 1 1 2 | 14.71 |
| 5.68 | 15 | 0 1 4 | 15.58 |
| 5.58 | 2 | -1 1 4 | 15.88 |
| 5.43 | 6 | -2 0 2 | 16.30 |
| 5.25 | 18 | 2 0 0 | 16.87 |
| 5.21 | 46 | 0 2 0 | 17.01 |
| 4.86 | 11 | 0 2 2 | 18.23 |
| 4.86 | 57 | -2 0 4 | 18.24 |
| 4.85 | 53 | -1 1 5 | 18.26 |
| 4.83 | 1 | -2 1 1 | 18.37 |
| 4.82 | 5 | -2 1 2 | 18.40 |
| 4.81 | 2 | 0 1 5 | 18.42 |
| 4.69 | 21 | 2 1 0 | 18.91 |
| 4.67 | 1 | 1 2 0 | 19.00 |
| 4.67 | 6 | -2 1 3 | 19.01 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 4.59 | 6 | -1 | 2 | 2 | 19.32 |
| 4.52 | 58 | 0 | 0 | 6 | 19.61 |
| 4.51 | 1 | 1 | 2 | 1 | 19.68 |
| 4.49 | 4 | 2 | 0 | 2 | 19.74 |
| 4.40 | 2 | -2 | 1 | 4 | 20.14 |
| 4.37 | 29 | -1 | 2 | 3 | 20.29 |
| 4.25 | 5 | -1 | 1 | 6 | 20.90 |
| 4.15 | 90 | 0 | 1 | 6 | 21.40 |
| 4.13 | 1 | 0 | 2 | 4 | 21.49 |
| 4.13 | 100 | 2 | 1 | 2 | 21.52 |
| 4.09 | 2 | -1 | 2 | 4 | 21.72 |
| 4.09 | 18 | -2 | 1 | 5 | 21.72 |
| 4.03 | 33 | -2 | 0 | 6 | 22.05 |
| 4.02 | 21 | 1 | 1 | 5 | 22.12 |
| 3.787 | 1 | 1 | 0 | 6 | 23.47 |
| 3.765 | 2 | -2 | 2 | 1 | 23.61 |
| 3.760 | 42 | -2 | 2 | 2 | 23.64 |
| 3.757 | 46 | -2 | 1 | 6 | 23.67 |
| 3.750 | 3 | -1 | 1 | 7 | 23.71 |
| 3.698 | 22 | 2 | 2 | 0 | 24.04 |
| 3.686 | 7 | -2 | 2 | 3 | 24.12 |
| 3.684 | 52 | 2 | 0 | 4 | 24.14 |
| 3.640 | 1 | 1 | 2 | 4 | 24.44 |
| 3.571 | 2 | 2 | 2 | 1 | 24.91 |
| 3.559 | 1 | 1 | 1 | 6 | 25.00 |
| 3.554 | 50 | -2 | 2 | 4 | 25.04 |
| 3.529 | 1 | -1 | 0 | 8 | 25.22 |
| 3.470 | 12 | -1 | 2 | 6 | 25.65 |
| 3.440 | 2 | -3 | 1 | 2 | 25.88 |
| 3.438 | 2 | -2 | 1 | 7 | 25.89 |
| 3.415 | 1 | 0 | 2 | 6 | 26.07 |
| 3.404 | 11 | -3 | 1 | 1 | 26.16 |
| 3.402 | 7 | 2 | 2 | 2 | 26.17 |
| 3.392 | 1 | 0 | 0 | 8 | 26.25 |
| 3.364 | 3 | 0 | 3 | 2 | 26.47 |
| 3.351 | 2 | -3 | 1 | 4 | 26.58 |
| 3.342 | 3 | -1 | 1 | 8 | 26.65 |
| 3.339 | 4 | 1 | 2 | 5 | 26.67 |
| 3.300 | 4 | -2 | 0 | 8 | 27.00 |
| 3.270 | 1 | -1 | 3 | 2 | 27.25 |
| 3.242 | 1 | 0 | 3 | 3 | 27.49 |
| 3.239 | 1 | 1 | 3 | 1 | 27.51 |
| 3.225 | 3 | 0 | 1 | 8 | 27.64 |
| 3.194 | 11 | 3 | 1 | 1 | 27.91 |
| 3.186 | 2 | -2 | 2 | 6 | 27.98 |
| 3.186 | 13 | 1 | 1 | 7 | 27.99 |
| 3.146 | 31 | -2 | 1 | 8 | 28.35 |
| 3.091 | 1 | 0 | 3 | 4 | 28.86 |
| 3.073 | 1 | -1 | 3 | 4 | 29.03 |
| 3.063 | 1 | 1 | 2 | 6 | 29.13 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 3.034 | 2 | 2 | 0 | 6 | 29.42 |
| 3.014 | 8 | 1 | 3 | 3 | 29.62 |
| 3.008 | 11 | 2 | 2 | 4 | 29.68 |
| 3.006 | 9 | -1 | 1 | 9 | 29.69 |
| 2.985 | 12 | -2 | 2 | 7 | 29.91 |
| 2.974 | 13 | -3 | 2 | 3 | 30.02 |
| 2.963 | 9 | -3 | 2 | 1 | 30.14 |
| 2.933 | 7 | -3 | 1 | 7 | 30.45 |
| 2.926 | 2 | -2 | 3 | 2 | 30.52 |
| 2.925 | 3 | 0 | 3 | 5 | 30.54 |
| 2.921 | 1 | -1 | 2 | 8 | 30.58 |
| 2.913 | 26 | 2 | 1 | 6 | 30.67 |
| 2.884 | 1 | -2 | 1 | 9 | 30.98 |
| 2.879 | 5 | 3 | 1 | 3 | 31.04 |
| 2.851 | 2 | -3 | 2 | 5 | 31.35 |
| 2.834 | 4 | 2 | 3 | 1 | 31.54 |
| 2.788 | 7 | -2 | 2 | 8 | 32.08 |
| 2.754 | 2 | 0 | 3 | 6 | 32.48 |
| 2.748 | 1 | 2 | 3 | 2 | 32.56 |
| 2.743 | 1 | -2 | 0 | 10 | 32.62 |
| 2.736 | 1 | -2 | 3 | 5 | 32.70 |
| 2.723 | 4 | -4 | 0 | 2 | 32.86 |
| 2.717 | 7 | -4 | 0 | 4 | 32.94 |
| 2.714 | 2 | 1 | 3 | 5 | 32.97 |
| 2.713 | 2 | 0 | 0 | 10 | 32.98 |
| 2.689 | 1 | -1 | 2 | 9 | 33.29 |
| 2.678 | 1 | 2 | 1 | 7 | 33.44 |
| 2.653 | 2 | -2 | 1 | 10 | 33.76 |
| 2.630 | 1 | -2 | 3 | 6 | 34.06 |
| 2.629 | 2 | -4 | 1 | 4 | 34.07 |
| 2.628 | 3 | -1 | 3 | 7 | 34.09 |
| 2.626 | 2 | 4 | 0 | 0 | 34.12 |
| 2.621 | 1 | 2 | 2 | 6 | 34.18 |
| 2.618 | 3 | 1 | 1 | 9 | 34.23 |
| 2.609 | 1 | 0 | 2 | 9 | 34.34 |
| 2.601 | 5 | -2 | 2 | 9 | 34.46 |
| 2.600 | 3 | -3 | 1 | 9 | 34.47 |
| 2.593 | 2 | 0 | 4 | 1 | 34.57 |
| 2.558 | 2 | 0 | 4 | 2 | 35.05 |
| 2.547 | 6 | 3 | 1 | 5 | 35.21 |
| 2.546 | 5 | 4 | 1 | 0 | 35.22 |
| 2.544 | 1 | 2 | 0 | 8 | 35.25 |
| 2.533 | 1 | -1 | 4 | 1 | 35.41 |
| 2.528 | 2 | 1 | 4 | 0 | 35.48 |
| 2.527 | 5 | 2 | 3 | 4 | 35.49 |
| 2.516 | 1 | -1 | 4 | 2 | 35.66 |
| 2.507 | 2 | -3 | 3 | 3 | 35.79 |
| 2.502 | 6 | 1 | 4 | 1 | 35.87 |
| 2.492 | 1 | -1 | 1 | 11 | 36.02 |
| 2.478 | 5 | -1 | 4 | 3 | 36.22 |

| Calculated Pattern (Integrated) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| 2.475 | 4 | -1 3 8 | 36.27 |
| 2.471 | 1 | 2 1 8 | 36.32 |
| 2.453 | 2 | 4 0 2 | 36.60 |
| 2.449 | 1 | -2 1 11 | 36.66 |
| 2.431 | 5 | 0 4 4 | 36.94 |
| 2.430 | 3 | -4 0 8 | 36.96 |
| 2.426 | 2 | 0 3 8 | 37.02 |
| 2.409 | 2 | 1 3 7 | 37.29 |
| 2.393 | 3 | 1 4 3 | 37.55 |
| 2.392 | 1 | -2 3 8 | 37.57 |
| 2.388 | 1 | 4 1 2 | 37.64 |
| 2.387 | 2 | -3 2 9 | 37.66 |
| 2.367 | 2 | -4 1 8 | 37.99 |
| 2.345 | 3 | 3 2 5 | 38.35 |
| 2.333 | 3 | -4 2 6 | 38.57 |
| 2.330 | 2 | -2 4 3 | 38.61 |
| 2.326 | 2 | -2 0 12 | 38.68 |
| 2.285 | 1 | 2 3 6 | 39.41 |
| 2.277 | 2 | 0 3 9 | 39.55 |
| 2.244 | 1 | 3 1 7 | 40.14 |
| 2.222 | 3 | -4 0 10 | 40.56 |
| 2.213 | 2 | 1 1 11 | 40.74 |
| 2.212 | 1 | -3 3 8 | 40.76 |
| 2.210 | 1 | 0 1 12 | 40.80 |
| 2.194 | 1 | 2 4 3 | 41.10 |
| 2.176 | 3 | 2 0 10 | 41.47 |
| 2.153 | 3 | -2 3 10 | 41.94 |
| 2.143 | 1 | 4 2 3 | 42.12 |
| 2.143 | 2 | -4 3 2 | 42.13 |
| 2.138 | 2 | -5 1 3 | 42.23 |
| 2.134 | 1 | 1 3 9 | 42.32 |
| 2.130 | 2 | 2 1 10 | 42.41 |
| 2.128 | 2 | -5 1 5 | 42.45 |
| 2.125 | 1 | -4 3 1 | 42.51 |
| 2.124 | 2 | -2 2 12 | 42.53 |
| 2.121 | 1 | -1 1 13 | 42.60 |
| 2.115 | 1 | -3 4 3 | 42.72 |
| 2.069 | 1 | -3 4 5 | 43.71 |
| 2.063 | 3 | 4 2 4 | 43.85 |
| 2.059 | 2 | 0 5 2 | 43.93 |
| 2.037 | 1 | -1 5 2 | 44.43 |
| 2.030 | 2 | 0 5 3 | 44.59 |
| 2.030 | 1 | -3 4 6 | 44.60 |
| 2.030 | 1 | 1 5 1 | 44.61 |
| 2.012 | 1 | 5 1 1 | 45.02 |
| 2.010 | 1 | -2 0 14 | 45.08 |
| 1.999 | 6 | 4 1 6 | 45.32 |
| 1.983 | 1 | -3 4 7 | 45.73 |
| 1.977 | 1 | -4 1 12 | 45.86 |
| 1.973 | 3 | -2 1 14 | 45.96 |

| Calculated Pattern (Integrated) | | | |
|---|---|---|---|
| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
| 1.947 | 1 | 4 3 3 | 46.60 |
| 1.941 | 1 | -3 0 14 | 46.77 |
| 1.938 | 2 | 0 0 14 | 46.84 |
| 1.933 | 1 | -2 3 12 | 46.98 |
| 1.928 | 1 | -3 4 8 | 47.09 |
| 1.919 | 1 | -3 2 13 | 47.33 |
| 1.917 | 2 | 3 3 7 | 47.39 |
| 1.902 | 1 | -1 5 6 | 47.79 |
| 1.890 | 3 | 2 5 2 | 48.10 |
| 1.886 | 1 | 4 3 4 | 48.21 |
| 1.882 | 1 | -4 4 2 | 48.31 |
| 1.878 | 1 | -4 2 12 | 48.42 |
| 1.872 | 1 | -5 2 9 | 48.60 |
| 1.863 | 2 | 2 1 12 | 48.84 |
| 1.858 | 2 | -3 3 12 | 48.98 |
| 1.844 | 1 | 2 3 10 | 49.39 |
| 1.843 | 1 | -1 1 15 | 49.42 |
| 1.842 | 1 | 4 0 8 | 49.44 |
| 1.822 | 2 | -5 3 1 | 50.01 |
| 1.801 | 1 | -3 1 15 | 50.64 |
| 1.796 | 1 | -3 5 4 | 50.81 |
| 1.794 | 1 | -1 5 8 | 50.85 |
| 1.794 | 1 | -4 1 14 | 50.86 |
| 1.791 | 1 | 1 4 10 | 50.96 |
| 1.780 | 1 | 2 2 12 | 51.29 |
| 1.777 | 1 | -4 4 8 | 51.38 |
| 1.775 | 2 | 0 5 8 | 51.43 |
| 1.774 | 2 | -3 3 13 | 51.46 |
| 1.770 | 2 | -6 0 8 | 51.60 |
| 1.750 | 1 | 6 0 0 | 52.22 |
| 1.744 | 1 | -3 4 11 | 52.42 |
| 1.740 | 1 | -2 1 16 | 52.57 |
| 1.737 | 1 | 4 2 8 | 52.66 |
| 1.723 | 1 | 3 4 7 | 53.10 |
| 1.711 | 1 | -6 2 6 | 53.52 |
| 1.709 | 1 | -4 1 15 | 53.58 |
| 1.694 | 1 | -3 3 14 | 54.09 |
| 1.671 | 1 | -2 2 16 | 54.90 |
| 1.668 | 1 | 4 0 10 | 54.99 |
| 1.665 | 1 | 2 5 7 | 55.10 |
| 1.659 | 1 | -2 5 10 | 55.32 |
| 1.655 | 1 | -1 6 5 | 55.46 |
| 1.653 | 1 | 0 5 10 | 55.56 |
| 1.588 | 1 | 4 5 2 | 58.03 |
| 1.550 | 1 | -4 3 15 | 59.58 |

# Silicon nitride, $\beta$-$Si_3N_4$

Structure
Hexagonal, $P6_3/m$ (176), Z = 4. The structure was determined by Hardie and Jack [1957].

Atom positions [ibid.]
6(h) 6 silicon
6(h) 6 nitrogen
2(c) 2 nitrogen

Polymorphism [ibid.]
A polymorph, $\alpha$-$Si_3N_4$ is also hexagonal, with space group P31c; its structure has the same tetrahedral units as the $\beta$ form but their arrangement is different.

Lattice constants
a = 7.608 A
c = 2.9109
(published values a = 7.608, c = 2.9107 [Hardie and Jack, 1957]).

CD cell; a = 7.608, c = 2.9109, c/a = 0.3826

Volume
145.9 $Å^3$

Density
(measured) 3.19 $g/cm^3$
(calculated) 3.193 $g/cm^3$

Thermal parameters
Isotropic: overall B = 0.5

Scattering factors
$Si^0$, $N^0$ [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 0.457 \times 10^{-3}$

Additional pattern
1. PDF card 9-259 [Decker, General Electric Co., Schenectady, N.Y.]

References
Hardie, D. and Jack, K. H. (1957). Nature, London, No. 4581, Aug. 17, p. 332.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

| d(Å) | I | hkl | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 6.58 | 40 | 1 0 0 | 13.44 |
| 3.80 | 40 | 1 1 0 | 23.38 |
| 3.29 | 100 | 2 0 0 | 27.06 |
| 2.66 | 95 | 1 0 1 | 33.64 |
| 2.49 | 95 | 2 1 0 | 36.04 |
| 2.31 | 6 | 1 1 1 | 38.94 |
| 2.20 | 5 | 3 0 0 | 41.08 |
| 2.18 | 35 | 2 0 1 | 41.36 |
| 1.902 | 8 | 2 2 0 | 47.78 |
| 1.892 | 5 | 2 1 1 | 48.04 |
| 1.827 | 12 | 1 3 0 | 49.86 |
| 1.753 | 35 | 3 0 1 | 52.14 |
| 1.592 | 11 | 2 2 1 | 57.86 |
| 1.548 | 6 | 1 3 1+ | 59.70 |
| 1.511 | 14 | 2 3 0+ | 61.28 |
| 1.455 | 14 | 0 0 2 | 63.92 |
| 1.438 | 7 | 1 4 0+ | 64.80 |
| 1.434 | 6 | 4 0 1 | 64.98 |
| 1.359 | 2 | 1 1 2 | 69.04 |
| 1.341 | 40 | 2 3 1 | 70.10 |
| 1.331 | 8 | 2 0 2 | 70.70 |
| 1.318 | 4 | 5 0 0 | 71.54 |
| 1.289 | 20 | 4 1 1 | 73.40 |
| 1.268 | 6 | 3 3 0 | 74.82 |
| 1.257 | 16 | 2 1 2 | 75.62 |
| 1.200 | 2 | 5 0 1 | 79.84 |
| 1.183 | 1 | 5 1 0+ | 81.22 |
| 1.156 | 2 | 2 2 2 | 83.58 |
| 1.145 | 3 | 2 4 1+ | 84.58 |
| 1.138 | 4 | 1 3 2 | 85.16 |
| 1.096 | 4 | 5 1 1 | 89.28 |
| 1.083 | 3 | 4 3 0 | 90.66 |
| 1.055 | 1 | 2 5 0 | 93.80 |
| 1.048 | 7 | 2 3 2+ | 94.58 |
| 1.023 | 4 | 1 4 2+ | 97.72 |
| 1.015 | 1 | 3 4 1 | 98.72 |
| 1.005 | 2 | 1 6 0 | 100.10 |
| .9919 | 3 | 2 5 1+ | 101.90 |
| .9769 | 3 | 5 0 2 | 104.10 |
| .9599 | 3 | 1 0 3 | 106.74 |
| .9560 | 5 | 3 3 2 | 107.36 |
| .9497 | 10 | 1 6 1+ | 108.40 |
| .9413 | 2 | 5 3 0 | 109.84 |
| .9307 | 2 | 2 0 3 | 111.72 |
| .9182 | 2 | 5 1 2+ | 114.06 |
| .9137 | 2 | 2 6 0+ | 114.92 |
| .9040 | 4 | 4 4 1 | 116.88 |
| .8956 | 2 | 7 0 1+ | 118.66 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 6.59 | 35 | 1 | 0 | 0 | 13.43 |
| 3.80 | 41 | 1 | 1 | 0 | 23.37 |
| 3.29 | 100 | 2 | 0 | 0 | 27.04 |
| 2.66 | 100 | 1 | 0 | 1 | 33.63 |
| 2.49 | 100 | 2 | 1 | 0 | 36.04 |
| 2.31 | 6 | 1 | 1 | 1 | 38.93 |
| 2.20 | 3 | 3 | 0 | 0 | 41.06 |
| 2.18 | 35 | 2 | 0 | 1 | 41.36 |
| 1.902 | 9 | 2 | 2 | 0 | 47.78 |
| 1.892 | 5 | 2 | 1 | 1 | 48.04 |
| 1.827 | 13 | 1 | 3 | 0 | 49.86 |
| 1.753 | 40 | 3 | 0 | 1 | 52.13 |
| 1.592 | 13 | 2 | 2 | 1 | 57.87 |
| 1.548 | 2 | 3 | 1 | 1 | 59.70 |
| 1.548 | 5 | 1 | 3 | 1 | 59.70 |
| 1.512 | 7 | 3 | 2 | 0 | 61.28 |
| 1.512 | 9 | 2 | 3 | 0 | 61.28 |
| 1.455 | 17 | 0 | 0 | 2 | 63.91 |
| 1.438 | 4 | 4 | 1 | 0 | 64.79 |
| 1.438 | 5 | 1 | 4 | 0 | 64.79 |
| 1.434 | 3 | 4 | 0 | 1 | 65.00 |
| 1.359 | 3 | 1 | 1 | 2 | 69.04 |
| 1.341 | 6 | 3 | 2 | 1 | 70.09 |
| 1.341 | 45 | 2 | 3 | 1 | 70.09 |
| 1.331 | 9 | 2 | 0 | 2 | 70.71 |
| 1.318 | 5 | 5 | 0 | 0 | 71.54 |
| 1.289 | 25 | 4 | 1 | 1 | 73.39 |
| 1.268 | 7 | 3 | 3 | 0 | 74.82 |
| 1.257 | 19 | 2 | 1 | 2 | 75.62 |
| 1.200 | 2 | 5 | 0 | 1 | 79.83 |
| 1.183 | 2 | 5 | 1 | 0 | 81.22 |
| 1.156 | 3 | 2 | 2 | 2 | 83.59 |
| 1.145 | 4 | 2 | 4 | 1 | 84.58 |
| 1.138 | 4 | 1 | 3 | 2 | 85.16 |
| 1.096 | 5 | 5 | 1 | 1 | 89.28 |
| 1.083 | 4 | 4 | 3 | 0 | 90.66 |
| 1.055 | 1 | 2 | 5 | 0 | 93.79 |
| 1.048 | 4 | 3 | 2 | 2 | 94.57 |
| 1.048 | 5 | 2 | 3 | 2 | 94.57 |
| 1.023 | 3 | 1 | 4 | 2 | 97.72 |
| 1.023 | 3 | 4 | 1 | 2 | 97.72 |
| 1.015 | 1 | 3 | 4 | 1 | 98.72 |
| 1.005 | 3 | 1 | 6 | 0 | 100.11 |
| .9919 | 1 | 5 | 2 | 1 | 101.90 |
| .9919 | 4 | 2 | 5 | 1 | 101.90 |
| .9768 | 5 | 5 | 0 | 2 | 104.11 |
| .9599 | 3 | 1 | 0 | 3 | 106.74 |
| .9560 | 6 | 3 | 3 | 2 | 107.36 |
| .9510 | 1 | 4 | 4 | 0 | 108.19 |
| .9498 | 10 | 1 | 6 | 1 | 108.39 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| .9498 | 4 | 6 | 1 | 1 | 108.39 |
| .9412 | 2 | 5 | 3 | 0 | 109.85 |
| .9307 | 3 | 2 | 0 | 3 | 111.72 |
| .9182 | 2 | 5 | 1 | 2 | 114.06 |
| .9137 | 3 | 2 | 6 | 0 | 114.93 |
| .9040 | 5 | 4 | 4 | 1 | 116.89 |
| .8956 | 1 | 5 | 3 | 1 | 118.66 |
| .8956 | 2 | 7 | 0 | 1 | 118.66 |

# Vanadium sulfide, $\alpha$-$V_3S$

Structure
Tetragonal, $I\bar{4}2m$ (121), Z = 8. The structure was determined by Pedersen and Grønvold [1959], and is closely related to that of $Ni_3P$.

Atom positions [ibid.]

| | | | |
|---|---|---|---|
| 8(i) | 8 vanadium(1) | 8(f) | 8 vanadium(3) |
| 8(i) | 8 vanadium(2) | 8(g) | 8 sulfur |

Polymorphism [ibid.]
The material was stable above 950 °C, and appeared also in samples quenched from 1400 °C. A tetragonal polymorph, $\beta$-$V_3S$ is stable below 825 °C, and has the space group $P4_2/nbc$. The structures are closely related.

Lattice constants [ibid.]
a = 9.470 A
c = 4.589

CD cell: a = 9.470, c = 4.589, c/a = 0.4846

Volume
411.6 $Å^3$

Density
(measured) 5.895 $g/cm^3$
(calculated) 5.968 $g/cm^3$

Thermal parameters
B = 0 since absorption and temperature effects nearly balance each other [Pedersen and Grønvold, 1959].

Scattering factors
$S^0$, $V^0$ [Cromer polynomial format: Cromer, 1972; Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.171 \times 10^{-3}$

References


Cromer, D. T. (1972). Private communication.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Pedersen, B. and Grønvold, F. (1959). Acta Crystallogr. 12, 1022.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 4.13 | 1 | 1 0 1 | 21.52 |
| 3.112 | 1 | 2 1 1 | 28.66 |
| 2.994 | 1 | 3 1 0 | 29.82 |
| 2.601 | 8 | 3 0 1 | 34.46 |
| 2.280 | 100 | 3 2 1 | 39.50 |
| 2.232 | 55 | 3 3 0 | 40.38 |
| 2.170 | 60 | 1 1 2 | 41.58 |
| 2.118 | 30 | 4 2 0 | 42.66 |
| 2.064 | 20 | 2 0 2 | 43.82 |
| 2.054 | 100 | 4 1 1 | 44.06 |

Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 1.892 | 40 | 2 2 2 | 48.04 |
| 1.857 | 16 | 5 1 0 | 49.02 |
| 1.821 | 12 | 3 1 2 | 50.04 |
| 1.751 | 7 | 4 3 1+ | 52.20 |
| 1.648 | 9 | 4 0 2 | 55.74 |
| 1.643 | 9 | 5 2 1 | 55.92 |
| 1.600 | 3 | 3 3 2 | 57.56 |
| 1.578 | 1 | 6 0 0 | 58.42 |
| 1.497 | 4 | 6 2 0 | 61.92 |
| 1.474 | 14 | 6 1 1 | 63.00 |
| 1.408 | 1 | 5 4 1 | 66.36 |
| 1.376 | 1 | 3 0 3 | 68.06 |
| 1.352 | 5 | 4 4 2 | 69.44 |
| 1.349 | 6 | 6 3 1 | 69.62 |
| 1.339 | 11 | 7 1 0+ | 70.22 |
| 1.326 | 9 | 5 3 2 | 71.06 |
| 1.322 | 17 | 3 2 3 | 71.28 |
| 1.313 | 3 | 6 4 0 | 71.82 |
| 1.300 | 10 | 6 0 2 | 72.66 |
| 1.2732 | 15 | 4 1 3 | 74.46 |
| 1.2515 | 10 | 7 2 1 | 75.98 |
| 1.2434 | 5 | 7 3 0 | 76.56 |
| 1.1900 | 2 | 4 3 3+ | 80.68 |
| 1.1722 | 3 | 6 5 1 | 82.16 |
| 1.1566 | 13 | 5 5 2 | 83.52 |
| 1.1472 | 8 | 0 0 4 | 84.36 |
| 1.1378 | 10 | 7 4 1 | 85.22 |
| 1.1160 | 2 | 6 6 0 | 87.30 |
| 1.1010 | 1 | 7 5 0 | 88.80 |
| 1.0911 | 5 | 6 1 3 | 89.82 |
| 1.0774 | 7 | 8 3 1 | 91.28 |
| 1.0521 | 6 | 8 0 2 | 94.14 |
| 1.0374 | 2 | 6 3 3 | 95.90 |
| 1.0269 | 3 | 8 2 2 | 97.20 |
| 1.0257 | 1 | 9 0 1 | 97.36 |
| 1.0203 | 6 | 3 3 4 | 98.04 |
| 1.0133 | 1 | 7 0 3 | 98.96 |
| 1.0087 | 4 | 4 2 4 | 99.58 |
| 1.0023 | 2 | 9 2 1+ | 100.44 |
| .9909 | 5 | 7 2 3 | 102.04 |
| .9806 | 2 | 8 5 1 | 103.54 |
| .9761 | 4 | 5 1 4 | 104.22 |
| .9515 | 3 | 9 1 2 | 108.10 |
| .9502 | 2 | 6 5 3 | 108.32 |
| .9470 | 5 | 10 0 0 | 108.86 |
| .9411 | 6 | 9 4 1 | 109.88 |
| .9317 | 6 | 7 4 3 | 111.54 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 4.13 | 1 | 1 | 0 | 1 | 21.50 |
| 3.112 | 1 | 2 | 1 | 1 | 28.66 |
| 2.995 | 1 | 3 | 1 | 0 | 29.81 |
| 2.601 | 8 | 3 | 0 | 1 | 34.46 |
| 2.294 | 1 | 0 | 0 | 2 | 39.23 |
| 2.280 | 100 | 3 | 2 | 1 | 39.50 |
| 2.232 | 55 | 3 | 3 | 0 | 40.38 |
| 2.171 | 60 | 1 | 1 | 2 | 41.57 |
| 2.118 | 30 | 4 | 2 | 0 | 42.66 |
| 2.065 | 14 | 2 | 0 | 2 | 43.81 |
| 2.054 | 100 | 4 | 1 | 1 | 44.05 |
| 1.893 | 40 | 2 | 2 | 2 | 48.03 |
| 1.857 | 17 | 5 | 1 | 0 | 49.01 |
| 1.821 | 13 | 3 | 1 | 2 | 50.04 |
| 1.751 | 3 | 5 | 0 | 1 | 52.21 |
| 1.751 | 4 | 4 | 3 | 1 | 52.21 |
| 1.648 | 9 | 4 | 0 | 2 | 55.75 |
| 1.642 | 6 | 5 | 2 | 1 | 55.95 |
| 1.600 | 3 | 3 | 3 | 2 | 57.56 |
| 1.578 | 1 | 6 | 0 | 0 | 58.42 |
| 1.497 | 4 | 6 | 2 | 0 | 61.92 |
| 1.474 | 16 | 6 | 1 | 1 | 63.00 |
| 1.408 | 1 | 5 | 4 | 1 | 66.35 |
| 1.377 | 1 | 3 | 0 | 3 | 68.05 |
| 1.352 | 5 | 4 | 4 | 2 | 69.44 |
| 1.349 | 4 | 6 | 3 | 1 | 69.62 |
| 1.339 | 7 | 7 | 1 | 0 | 70.22 |
| 1.339 | 5 | 5 | 5 | 0 | 70.22 |
| 1.326 | 10 | 5 | 3 | 2 | 71.05 |
| 1.322 | 14 | 3 | 2 | 3 | 71.29 |
| 1.313 | 2 | 6 | 4 | 0 | 71.83 |
| 1.300 | 11 | 6 | 0 | 2 | 72.65 |
| 1.2976 | 2 | 7 | 0 | 1 | 72.83 |
| 1.2732 | 18 | 4 | 1 | 3 | 74.46 |
| 1.2540 | 1 | 6 | 2 | 2 | 75.80 |
| 1.2515 | 11 | 7 | 2 | 1 | 75.98 |
| 1.2435 | 5 | 7 | 3 | 0 | 76.56 |
| 1.1900 | 1 | 5 | 0 | 3 | 80.68 |
| 1.1900 | 1 | 4 | 3 | 3 | 80.68 |
| 1.1723 | 4 | 6 | 5 | 1 | 82.16 |
| 1.1566 | 15 | 5 | 5 | 2 | 83.51 |
| 1.1541 | 2 | 5 | 2 | 3 | 83.74 |
| 1.1472 | 9 | 0 | 0 | 4 | 84.36 |
| 1.1398 | 2 | 6 | 4 | 2 | 85.04 |
| 1.1379 | 11 | 7 | 4 | 1 | 85.21 |
| 1.1161 | 2 | 6 | 6 | 0 | 87.29 |
| 1.1009 | 1 | 7 | 5 | 0 | 88.81 |
| 1.0911 | 5 | 6 | 1 | 3 | 89.82 |
| 1.0774 | 9 | 8 | 3 | 1 | 91.28 |
| 1.0520 | 7 | 8 | 0 | 2 | 94.15 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.0374 | 2 | 6 | 3 | 3 | 95.89 |
| 1.0270 | 3 | 8 | 2 | 2 | 97.19 |
| 1.0256 | 1 | 9 | 0 | 1 | 97.37 |
| 1.0204 | 8 | 3 | 3 | 4 | 98.04 |
| 1.0134 | 1 | 7 | 0 | 3 | 98.95 |
| 1.0087 | 5 | 4 | 2 | 4 | 99.57 |
| 1.0024 | 2 | 9 | 2 | 1 | 100.44 |
| 1.0024 | 1 | 7 | 6 | 1 | 100.44 |
| .9909 | 6 | 7 | 2 | 3 | 102.03 |
| .9806 | 2 | 8 | 5 | 1 | 103.54 |
| .9760 | 5 | 5 | 1 | 4 | 104.22 |
| .9516 | 4 | 9 | 1 | 2 | 108.09 |
| .9502 | 2 | 6 | 5 | 3 | 108.32 |
| .9470 | 6 | 10 | 0 | 0 | 108.86 |
| .9411 | 8 | 9 | 4 | 1 | 109.87 |
| .9316 | 8 | 7 | 4 | 3 | 111.55 |

# Vanadium sulfide, $\beta$-$V_3S$

Structure
Tetragonal, $P4_2/nbc$ (133), Z = 8. The structure was determined by Pedersen and Grønvold [1959] and shows relationship to the $\beta$-W structure type.

Atom positions [ibid.]

| | | | |
|---|---|---|---|
| 8(j) | 8 vanadium(1) | 8(i) | 8 vanadium(3) |
| 8(j) | 8 vanadium(2) | 8(h) | 8 sulfur |

Polymorphism [ibid.]
The material was stable below 825 °C. A tetragonal polymorph, $\alpha$-$V_3S$ has the space group $I\bar{4}2m$; it is stable above 950 °C and appears also in samples quenched from 1400 °C. The two structures are closely related.

Lattice constants [ibid.]
a = 9.381 A
c = 4.663

CD cell: a = 9.381, c = 4.663, c/a = 0.4971

Volume
410.4 $Å^3$

Density
(measured) 5.939 $g/cm^3$
(calculated) 5.985 $g/cm^3$

Thermal parameters
B = 0, since absorption and temperature effects nearly balance each other [Pedersen and Grønvold, 1959].

Scattering factors
$V^0$, $S^0$, [Cromer polynomial format: Cromer, 1972; Cromer and Mann, 1968].

Scale factors (integrated intensities)
$\gamma = 0.152 \times 10^{-3}$

References


Cromer, D. T. (1972). Private communication.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Pedersen, B. and Grønvold, F. (1959). Acta Crystallogr. 12, 1022.


Calculated Pattern (Peak heights)

| d(Å) | I | hkℓ | 2θ(°) λ = 1.540598Å |
|---|---|---|---|
| 2.502 | 25 | 3 1 1 | 35.86 |
| 2.345 | 2 | 4 0 0 | 38.36 |
| 2.332 | 2 | 0 0 2 | 38.58 |
| 2.272 | 100 | 3 2 1 | 39.64 |
| 2.211 | 60 | 3 3 0 | 40.78 |
| 2.200 | 75 | 1 1 2 | 41.00 |
| 2.097 | 45 | 4 2 0+ | 43.10 |
| 2.045 | 75 | 4 1 1 | 44.26 |
| 1.913 | 30 | 4 2 1 | 47.50 |
| 1.907 | 60 | 2 2 2 | 47.64 |
| 1.840 | 20 | 5 1 0 | 49.50 |
| 1.834 | 19 | 3 1 2 | 49.68 |
| 1.711 | 6 | 5 1 1 | 53.50 |
| 1.653 | 9 | 4 0 2 | 55.54 |
| 1.605 | 4 | 3 3 2 | 57.38 |
| 1.483 | 4 | 6 2 0+ | 62.58 |
| 1.464 | 15 | 6 1 1 | 63.48 |
| 1.414 | 1 | 6 2 1 | 66.04 |
| 1.398 | 1 | 5 4 1 | 66.88 |
| 1.377 | 2 | 3 1 3 | 68.04 |
| 1.351 | 4 | 4 4 2 | 69.50 |
| 1.339 | 2 | 6 3 1 | 70.22 |
| 1.334 | 14 | 3 2 3 | 70.52 |
| 1.326 | 13 | 7 1 0+ | 71.00 |
| 1.324 | 14 | 5 3 2 | 71.16 |
| 1.2984 | 14 | 6 0 2 | 72.78 |
| 1.2953 | 10 | 4 0 3 | 72.98 |
| 1.2835 | 12 | 4 1 3 | 73.76 |
| 1.2761 | 3 | 7 1 1 | 74.26 |
| 1.2531 | 9 | 6 4 1 | 75.86 |
| 1.2498 | 7 | 4 2 3 | 76.10 |
| 1.2420 | 6 | 7 2 1 | 76.66 |
| 1.2317 | 5 | 7 3 0 | 77.42 |
| 1.1910 | 7 | 7 3 1 | 80.60 |
| 1.1878 | 5 | 5 1 3 | 80.86 |
| 1.1657 | 9 | 0 0 4 | 82.72 |
| 1.1530 | 15 | 5 5 2 | 83.84 |
| 1.1361 | 2 | 6 4 2 | 85.38 |
| 1.1055 | 2 | 6 6 0 | 88.34 |
| 1.0947 | 5 | 6 1 3 | 89.44 |
| 1.0907 | 1 | 7 5 0 | 89.86 |
| 1.0687 | 8 | 8 3 1 | 92.24 |
| 1.0619 | 5 | 7 5 1 | 93.00 |
| 1.0476 | 6 | 8 0 2 | 94.66 |
| 1.0312 | 7 | 3 3 4 | 96.66 |
| 1.0231 | 4 | 8 4 1 | 97.68 |
| 1.0225 | 4 | 8 2 2 | 97.76 |
| 1.0190 | 6 | 4 2 4 | 98.22 |
| 1.0114 | 2 | 9 1 1 | 99.22 |
| 1.0090 | 2 | 7 1 3 | 99.54 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 2.503 | 20 | 3 | 1 | 1 | 35.85 |
| 2.345 | 2 | 4 | 0 | 0 | 38.35 |
| 2.331 | 1 | 0 | 0 | 2 | 38.58 |
| 2.272 | 100 | 3 | 2 | 1 | 39.64 |
| 2.211 | 55 | 3 | 3 | 0 | 40.78 |
| 2.200 | 65 | 1 | 1 | 2 | 41.00 |
| 2.098 | 35 | 4 | 2 | 0 | 43.09 |
| 2.095 | 16 | 4 | 0 | 1 | 43.14 |
| 2.088 | 16 | 2 | 0 | 2 | 43.30 |
| 2.045 | 75 | 4 | 1 | 1 | 44.26 |
| 1.913 | 20 | 4 | 2 | 1 | 47.49 |
| 1.907 | 55 | 2 | 2 | 2 | 47.64 |
| 1.840 | 20 | 5 | 1 | 0 | 49.50 |
| 1.833 | 13 | 3 | 1 | 2 | 49.70 |
| 1.711 | 7 | 5 | 1 | 1 | 53.50 |
| 1.653 | 9 | 4 | 0 | 2 | 55.53 |
| 1.604 | 5 | 3 | 3 | 2 | 57.39 |
| 1.483 | 4 | 6 | 2 | 0 | 62.57 |
| 1.482 | 1 | 6 | 0 | 1 | 62.62 |
| 1.464 | 17 | 6 | 1 | 1 | 63.48 |
| 1.413 | 1 | 6 | 2 | 1 | 66.04 |
| 1.398 | 1 | 5 | 4 | 1 | 66.89 |
| 1.377 | 3 | 3 | 1 | 3 | 68.04 |
| 1.351 | 5 | 4 | 4 | 2 | 69.50 |
| 1.339 | 1 | 6 | 3 | 1 | 70.21 |
| 1.334 | 15 | 3 | 2 | 3 | 70.52 |
| 1.327 | 8 | 7 | 1 | 0 | 70.99 |
| 1.327 | 5 | 5 | 5 | 0 | 70.99 |
| 1.324 | 10 | 5 | 3 | 2 | 71.14 |
| 1.301 | 3 | 6 | 4 | 0 | 72.62 |
| 1.2985 | 15 | 6 | 0 | 2 | 72.77 |
| 1.2956 | 3 | 4 | 0 | 3 | 72.96 |
| 1.2834 | 14 | 4 | 1 | 3 | 73.77 |
| 1.2760 | 3 | 7 | 1 | 1 | 74.27 |
| 1.2531 | 10 | 6 | 4 | 1 | 75.87 |
| 1.2515 | 1 | 6 | 2 | 2 | 75.98 |
| 1.2488 | 5 | 4 | 2 | 3 | 76.17 |
| 1.2420 | 7 | 7 | 2 | 1 | 76.66 |
| 1.2318 | 6 | 7 | 3 | 0 | 77.42 |
| 1.1909 | 8 | 7 | 3 | 1 | 80.60 |
| 1.1873 | 2 | 5 | 1 | 3 | 80.90 |
| 1.1657 | 10 | 0 | 0 | 4 | 82.72 |
| 1.1531 | 18 | 5 | 5 | 2 | 83.83 |
| 1.1360 | 2 | 6 | 4 | 2 | 85.38 |
| 1.1056 | 3 | 6 | 6 | 0 | 88.33 |
| 1.0948 | 6 | 6 | 1 | 3 | 89.44 |
| 1.0905 | 1 | 7 | 5 | 0 | 89.88 |
| 1.0687 | 9 | 8 | 3 | 1 | 92.23 |
| 1.0619 | 6 | 7 | 5 | 1 | 93.01 |
| 1.0476 | 7 | 8 | 0 | 2 | 94.67 |

| Calculated Pattern (Integrated) | | | | | |
|---|---|---|---|---|---|
| d(Å) | I | hkℓ | | | 2θ(°) λ = 1.540598Å |
| 1.0312 | 9 | 3 | 3 | 4 | 96.66 |
| 1.0233 | 3 | 8 | 4 | 1 | 97.66 |
| 1.0224 | 3 | 8 | 2 | 2 | 97.78 |
| 1.0190 | 6 | 4 | 2 | 4 | 98.22 |
| 1.0113 | 3 | 9 | 1 | 1 | 99.23 |
| 1.0091 | 2 | 7 | 1 | 3 | 99.52 |

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Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the cumulative index here is not necessarily the concluding index for the project.

m - Monograph 25.

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*Natural mineral.

NBS-114A (REV. 7-73)

| U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET | 1. PUBLICATION OR REPORT NO. NBS MN-25, Section 14 | 2. Gov't Accession No. | 3. Recipient's Accession No. |
|---|---|---|---|

**4. TITLE AND SUBTITLE**

Standard X-ray Diffraction Powder Patterns
Section 14 -- Data for 68 Substances

**5. Publication Date**
September 1977

**6. Performing Organization Code**


**7. AUTHOR(S)** M. C. Morris, H. F. McMurdie, E. H. Evans, B. Paretzkin, J. H. de Groot, R. J. Newberry, C. R. Hubbard, S. J. Carmel

**8. Performing Organ. Report No.**

**9. PERFORMING ORGANIZATION NAME AND ADDRESS**

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

Joint Committee on
Powder Diffraction Standards
Swarthmore, PA 19081


**10. Project/Task/Work Unit No.**

**11. Contract/Grant No.**

**12. Sponsoring Organization Name and Complete Address (Street, City, State, ZIP)**

Same as 9.

**13. Type of Report & Period Covered**
Interim

**14. Sponsoring Agency Code**

**15. SUPPLEMENTARY NOTES**

Library of Congress Catalog Card Number: 53-61386


**16. ABSTRACT** *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

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UNCLASSIFIED

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143

**20. SECURITY CLASS (THIS PAGE)**
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**22. Price**
$2.75

USCOMM-DC 29042-P74


☆U.S. GOVERNMENT PRINTING OFFICE: 1977-240-848/320

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